MASTER

Towards BEC of metastable neon

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Towards BEC of metastable neon

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Summary

This thesis reports the progress made during the past year towards realizing a Bose-Einstein Condensate (BEC) of metastable neon atoms, a feat that no one has accomplished so far. To observe BEC experimentally, the metastable atoms need to be trapped and cooled to ultra cold temperatures (∼ 1μK) in a two-step process. First the atoms are loaded into a Magneto-Optical Trap (MOT), where temperatures of the order of 40 μK can be reached using laser cooling. From there, the atoms are further cooled in a Magneto-Static trap (MT) with forced evaporative cooling until BEC is realized. These traps must meet specific requirements. In addition, the possibility of reaching BEC is determined by the sign and magnitude of the scattering length, which characterizes elastic collisions between the trapped atoms at low temperatures. Only if the scattering length is positive, is a stable condensate possible. Furthermore, the efficiency of evaporative cooling used to reach BEC, is directly proportional to the scattering length squared.

The research described in this report consists of three parts. First the magnetic fields of the experimental realization of the MT and MOT are studied in detail. From measurements, we conclude that the traps meet the trapping requirements. During the transfer from MOT to MT, a weak cylindrical symmetric trapping potential with radial and axial trapping frequencies $\omega_r = \omega_z = 48 (2\pi)$ Hz can be accomplished. During the evaporative cooling phase, a tight confinement can be achieved with trapping frequencies $\omega_r/10 = \omega_z = 48 (2\pi)$ Hz. Essential is the existence of a small, positive minimum magnetic field during the latter phase. A minimum magnetic field of +1.7 G has been observed.

Second, a MOT has been realized experimentally and the first measurements of its performance are presented. The largest number of particles observed experimentally was $5 \times 10^8$ atoms, in a typical volume of 0.02 cm$^3$ at a typical particle density of $3 \times 10^{10}$ cm$^{-3}$. The lifetime of the trapped particles in the MOT due to ionization is of the order of 30 ms, long enough to cool the atom and to successively transfer them to the MT. The MOT needs to be optimized further to obtain the desired number of trapped particles ($10^{10}$ atoms) and MOT volume (0.1 cm$^3$).

Third, calculations of the scattering length and of photo-association (PA) spectra are carried out. Photo-association spectroscopy (PAS) is an experimental technique, which yields information on the scattering length and other collision parameters. From these calculations we conclude that there is only a 10 % probability that the scattering length is negative for both $^{20}$Ne* and its isotope $^{22}$Ne*. Therefore, the prospects are promising that BEC is possible for at least one of the two metastable neon isotopes.

The calculated PA spectra provide insight into how the value of the scattering length is reflected in (future) experimental PA spectra. In addition, they predict the absolute value of experimental signals, from which it can be concluded that PAS is well feasible.
Without wanting to derogate from somebody’s merits, I would like to thank some people in person, who helped realizing this thesis in a direct or indirect way.

First of all, I would like to thank my supervisor Edgar Vredenbregt, who always made time to answer my silly questions, for his guidance. Also, I would like to thank Sjef Tempelaars, who must know this thesis by heart by now. Herman Beijerinck, I would like to thank for preventing me from writing a handbook about laser cooling and trapping of atoms instead of a graduation report (although he might think he failed after all, reading this report). The other members of the Group of Theoretical and Experimental Atomic Physics and Quantum Electronics, I would like to thank for the nice and constructive cooperation. In particular, I want to name, Simon Kuppens and Boudewijn Verhaar. I’m grateful to Louis van Moll and especially Rien de Koning for teaching me some mechanical skills.

For lending me their three-dimensional manipulator and lab-space to perform my magnetic field measurements, the group of Physical Instrumentation and Clinical Physics (FIK), especially Jaap Feijen en Jef Noijen, earns my thanks.

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Chapter 1

Introduction

1.1 Introduction

In the group of Theoretical and Experimental Atomic Physics and Quantum Electronics of the Physics Department of the Eindhoven University of Technology, efforts are currently being made to realize a metastable neon Bose-Einstein Condensate, a feat that has not been accomplished so far. This thesis reports the progress being made during the past year towards this goal.

1.2 Bose-Einstein Condensation

Bose-Einstein Condensation (BEC) occurs when the mean distance between atoms is of the same order of magnitude as their thermal De Broglie wavelength $\Lambda$. This means that BEC only takes place at high phase space density $D$, in practice corresponding to extremely low temperatures. The phase space density is defined as:

$$D = n\Lambda^3,$$

(1.1)

where $n$ is the particle density, $\Lambda = (2\pi\hbar^2/mk_BT)^{1/2}$ the thermal De Broglie wavelength, $\hbar$ the constant of Dirac, $m$ the atomic mass, $k_B$ the Boltzmann constant and $T$ the temperature. Bose-Einstein Condensation occurs when

$$D \approx 2.61,$$

(1.2)

for example at a transition temperature $T_C = 1.7\,\mu\text{K}$ and a density $n = 10^{14}\,\text{cm}^{-3}$ for metastable neon. For temperatures below the BEC transition temperature $T_C$, (a fraction of) the atoms occupy a single macroscopic quantum state.

1.3 Metastable neon

Rare gases are of special interest because they are model atomic systems, which play an important role in both fundamental atomic physics and technological applications. Despite this, cold collisions of rare gas atoms have, until recently, not been the subject of study, contrary to such collisions among the alkali-metal gas atoms. This is probably due to the experimental difficulties involved in trapping
and cooling rare gas atoms as opposed to the relative experimental ease with which alkali-metal atoms can be manipulated. Excitation of rare gas atoms from the ground state to the first excited states via optical transitions is very difficult since extreme-ultraviolet lasers are required, which are not yet available.

However, some of the first excited states \((n-1)p^5n_s\) of the rare gas atoms are metastable and can be used as 'ground' state atoms in laser cooling processes. Here \(n\) is a quantum number, which gives the valence electron shell. For metastable neon \(n = 3\). From here optical transitions to the second excited states \((n-1)p^5np\) are possible. The long but still finite lifetime of the metastable rare gas atoms limits, however, the time scale of the experiments. In addition, the production efficiency of metastable rare gas atoms is very low \((\sim 10^{-4})\). Therefore, techniques of beam brightening and slowing of metastable atoms must be applied to obtain sufficient atoms to load an atomic trap. This leads to a rather complicated experimental setup (§ 3.4). Another disadvantage of the rare gas atoms is that Penning ionization of two colliding metastable rare gas atoms leads to loss of atoms from the trap. Fortunately, ionization might be strongly suppressed for all rare gas atoms except xenon, by spin polarizing the trapped atoms [4]. And last but not least, almost no theoretical or experimental data on binary atomic collisions and the interaction potentials of the rare gas atoms are available, except for helium.

In this report the first steps towards a BEC of metastable neon are taken. Why would we bother to go through so many difficulties to make a neon BEC? As mentioned above, the rare gas atoms are model atomic systems and therefore of special interest. Moreover, having a condensate of electronically excited atoms might yield a whole range of new possibilities. Collective phenomena in a condensate with a large electronic energy like collective electronic deexcitation might occur. In addition, the real time diagnostics for detecting metastable neon atoms are quite good, because the metastable atom emits UV photons and produces ions in ionizing collisions. Another advantage of metastable neon over the alkali-metal atoms, is its large magnetic moment, \(I_l = 3I_lB\), where \(I_lB\) is the Bohr magneton. As a result, far smaller magnetic fields are necessary to trap and cool the metastable neon atoms as compared to the alkali-metal atoms.

Figure 1.1 shows the level diagram of neon. Four first excited fine-structure states with electronic configuration \({(2p^5)(3s)}\) exist. Of these only the \(5^3P_0\) and the \(3^3P_2\) states are metastable, and have a lifetime of, respectively 430 and 24.4 s. The atomic states are given in Russell-Saunders notation: \(2S+1L_J\), where \(S\) is the total electron spin, \(L\) the total electronic orbital angular momentum and \(J\) the total electronic angular momentum. Only the \(5^3P_0\) state is both metastable and has nonzero angular momentum, allowing for magnetic trapping and spin polarization. Together with the second excited \(3D_3\) state, it forms a closed transition which can be used as laser cooling transition. The \(3D_3\) second excited state has electronic configuration \({(2p^5)(3p)}\) and a life time of 19.4 ns.

Neon has two suitable bosonic isotopes, \(^{20}\text{Ne}\) and \(^{22}\text{Ne}\), with respective natural abundances 90.9% and 9%. In chapters 2 and 3, only \(^{20}\text{Ne}\) is considered. In chapter 4, however, also \(^{22}\text{Ne}\) is considered, since we also plan to make a BEC of this less abundant isotope of neon in the future.

1.4 The road to BEC

In order to realize Bose Einstein condensation of metastable neon, first the atoms are cooled to low velocities, using laser cooling techniques. Second, these slow atoms are trapped in a Magneto-
Figure 1.1: Level diagram of the first and second excited states of neon. The metastable states are respectively $^3P_0$ and $^3P_2$. The other excited state of interest is $^3D_3$. The electronic configuration of the first and second excited states are respectively $(1s)^2(2s)^2(2p)^53s$ and $(1s)^2(2s)^2(2p)^53p$. The levels are given in Russell-Saunders notation. The cycling transition $\text{Ne}^*[^3P_2] \leftrightarrow \text{Ne}^{**}[^3D_3]$ forms the laser cooling cycle and is indicated.

Table 1.1: Characteristic quantities of the neon atom and the laser cooling transition $\text{Ne}^*[^3P_2] \leftrightarrow \text{Ne}^{**}[^3D_3]$.

<table>
<thead>
<tr>
<th>Quantity</th>
<th>Symbol</th>
<th>Value</th>
</tr>
</thead>
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<tr>
<td>Atomic Mass</td>
<td>$m$</td>
<td>$33.2 \times 10^{-27}$ kg</td>
</tr>
<tr>
<td>Wavelength</td>
<td>$\lambda$</td>
<td>640.225 nm</td>
</tr>
<tr>
<td>Wavenumber</td>
<td>$k = 2\pi/\lambda$</td>
<td>$9.81 \times 10^6$ m$^{-1}$</td>
</tr>
<tr>
<td>Internal energy of $^3P_2$ state</td>
<td>$E_i$</td>
<td>16.6 eV</td>
</tr>
<tr>
<td>Spontaneous decay rate</td>
<td>$\Gamma$</td>
<td>8.20($2\pi$) MHz</td>
</tr>
<tr>
<td>Natural lifetime</td>
<td>$\tau = 1/\Gamma$</td>
<td>19.4 ns</td>
</tr>
<tr>
<td>Magnetic moment</td>
<td>$\mu = 3\mu_B$</td>
<td>$2.78 \times 10^{-23}$ Am$^2$</td>
</tr>
</tbody>
</table>
Optical Trap (MOT) and cooled to even lower temperatures. Third, the atoms are transferred to a Magnetostatic Trap (MT) to cool them to temperatures below the BEC transition temperature.

Since BEC takes place at such low temperatures and such high particle densities, a very cold source of atoms with a high enough intensity is required to load an atom trap. Because metastable neon has an electronic energy of 16.6 eV, the relative population in a gas discharge or atomic beam is only \(10^{-4}\) of the total density. Therefore, beam brightening techniques must be applied to obtain sufficiently large fluxes of metastable neon atoms.

The purpose of the Gemini beamline (§ 3.4) is to provide such a source of metastable neon atoms. This cold atomic beam, with a typical initial temperature of 25 mK \((v_{\text{axial}} = 5 \text{ m/s})\) and a typical particle density of \(10^9 \text{ cm}^{-3}\), is then loaded into a Magneto-optical Trap (MOT). The phase space density of the beam is \(D = 1.5 \times 10^{-11}\).

In the optimum situation, the atoms in the MOT can be cooled to an equilibrium temperature of the order of \(T \approx 40 \mu\text{K}\). Assuming a typical MOT density of \(10^{11} \text{ cm}^3\), we can obtain a phase space density of \(D = 2.4 \times 10^{-5}\) in the MOT. So, we can realize an increase by a factor of \(10^6\) in the phase space density in the MOT.

In order to increase the phase space density to the critical value of 2.61, the atoms are further cooled in a Magnetostatic Trap (MT), using evaporative cooling. Both the MOT and the MT are briefly described in the next subsections.

### 1.4.1 The Magneto-optical Trap

Figure 1.2 shows a schematic picture of the principle of the Magneto-optical Trap (MOT). The MOT consists of three orthogonal pairs of red-detuned, counter propagating, circularly polarized laser beams and a pair of coils with equal, opposed currents. The laser beams are aligned along three mutually perpendicular axes. Of each pair of these laser beams one consists of \(\sigma^+\) light and the other of \(\sigma^-\) light. The so-called anti-Helmholtz coils generate a spherical quadrupole magnetic field. The combination of the quadrupole field and the laser beam configuration results in a trapping force for all directions in space to the origin, described in detail in § 3.2.

### 1.4.2 The Magnetostatic Trap

In order to trap atoms with a static potential \(U(r)\) around \(r = 0\), first, the trapping force, \(\vec{F} = -\nabla U\), should vanish at the center of the trap \((r = 0)\) and secondly, a restoring force should push displaced atoms back to the center of the trap. Or in formula [34]:

\[
\nabla U(0) = 0, \quad \nabla^2 U(0) > 0.
\]

In potentials that obey Laplace's equation, \(\nabla^2 U = 0\), no stable equilibrium exists and as a consequence trapping is not possible. This is the case for atoms precessing according to the Larmor frequency in an external homogeneous magnetic field.

In an inhomogeneous magnetic field, however, the energy levels of an atom depend on the spatial coordinates, due to the Zeeman effect. The Zeeman splitting of the energy levels is given by [14]:

\[
\Delta E = -\vec{\mu} \cdot \vec{B}_{\text{ext}} = m J \mu_B g_J B_{\text{ext}},
\]
in an external magnetic field aligned along the quantization axis. In this equation $m_J$ is the azimuthal quantum number, $\mu_B$ the Bohr magneton, $g_J$ the Landé g-factor and $m$ the atomic mass. As a result, the energy levels of an atom in an inhomogeneous static magnetic field $E_n(\vec{r})$ are position-dependent, leading to an external force $F_n = \nabla (\mu_B \cdot \vec{B}) = -\nabla E_n(\vec{r}) = -m_J \mu_B g_J \nabla B_{ext}$. In general these position-dependent energy levels do not obey Laplace's equation. Therefore, trapping of atoms in a static inhomogeneous magnetic field is possible.

Wing's proof states that the strength of a magnetic field in free space can have local minima but not local maxima [40]. As a consequence, stable trapping is only possible for atoms in the low-field seeking states with $m_J > 0$, around a local minimum in the magnetic field. Both the MOT and the MT provide such trapping fields.

The atoms moving around the MT perceive a continuously changing magnetic field. If the characteristic frequency of this variation is comparable to the Larmor frequency, the atoms can make so-called Majorana (spin flip) transitions to non-trapped states. This happens when the atoms are confined around a field minimum of $|B|_{min} = 0$ G, in other words in a quadrupole field of an anti-Helmholtz coil configuration. This problem can be avoided, however, when adding a bias magnetic field so that $|B_{min}| > 0$.

1.4.3 Evaporative cooling

Evaporative cooling

In order to increase the phase space density to the critical value where BEC takes place (1.2), evaporative cooling is used to cool the trapped atoms to temperatures below the critical BEC transition.
Evaporative cooling relies on the spatial selection of energetic particles and successively removing them from the trap.

The advantage of evaporative cooling is that it is a relatively simple process which is applicable to atomic gases with a wide range of temperatures and densities, and has the potential to cool atoms below temperatures that are attainable with other cooling methods. A disadvantage of evaporative cooling is the loss of atoms from the trap. Therefore the objective of evaporative cooling is a maximum increase in phase space density while minimizing the loss in the number of trapped atoms.

Evaporation of atoms is controlled by limiting the trap depth of the trapping potential to $\eta k_B T$, where $\eta$ is a positive number ($\sim 3 - 6$). All particles with an energy larger than $\eta k_B T$ leave the trap, resulting in a truncated Maxwell-Boltzmann distribution. Since the evaporated atoms take away more than the average energy per particle, the energy per trapped atom decreases. Then, the remaining atoms re-thermalize by elastic interatomic collisions. As a consequence, the average temperature of the trapped atoms drops.

In order to sustain evaporation, it is important to maintain or increase the elastic collision rate. The characteristic parameter for evaporative cooling is therefore the number of elastic collisions per trapping time, which is defined as [17]:

$$R = \tau_{loss} \nu_{el}. \quad (1.5)$$

Here $\tau_{loss}$ is the time constant for trap loss and $\nu_{el}$ the collision frequency for elastic collisions. The relative increase in phase space density with decreasing number of trapped atoms is maximum if $R$ is maximum.

A prerequisite for evaporative cooling is a large enough scattering length, so that the atoms re-thermalize easily and quickly through elastic collisions. The scattering length $a$ is a characteristic parameter for the interaction between two atoms at low collision energy, which determines the elastic collision cross section $\sigma_{el} = 8\pi a^2$. The elastic collision frequency is proportional to this elastic collision cross section: $\nu_{el} = n\sigma_{el}v$. A sufficiently large value of $a$ is essential for an effective cooling process. The scattering length will be discussed in more detail in Chapter 4.

A tight magnetic confinement or adiabatic compression, which can be achieved by increasing the strength of the magnetic trapping field, enhances the elastic collision rate $\nu_{el}$ and therefore the process of evaporative cooling. Adiabatic compression increases both temperature and density and therefore always increases $R$ and the speed of evaporative cooling. Phase space density stays constant. The ratio $R$ for collisions with the background gas increases, however, as well. For ionization, which also depend on the trap density, on the other hand, the value of $R$ remains constant [3]. Therefore, runaway cooling, as observed for the alkali-metal gases, does not occur in trapped metastable rare gas atoms.

Rf-induced evaporation

The MT can be used to cool atoms to extremely low temperatures by radiofrequency-induced evaporation. In radiative evaporation a rf field is used to transfer atoms from a trapped to an untrapped state in an energy-selective way. Since the magnetic field is minimum at the center of the trap, only weak-field seeking atoms with $m_J > 0$ are trapped. An atom will seek to lower its energy. The energy of weak-field seeking atoms increases with increasing magnetic field. Therefore weak-field seeking atoms will concentrate at the magnetic field minimum. Strong-field seeking atoms, however, are pushed out of the trap. To transfer the metastable neon atoms to these so-called trapped states, they are spin-polarized to the $^3P_2, m_J = 2 >$ state. To induce evaporative cooling, rf-radiation is used to flip
1.5 Heating and loss processes in metastable neon traps

Essential in trapping and cooling atoms to the ultra-low temperatures where Bose-Einstein Condensation (BEC) takes place (1 \( \mu \)K to 10 nK), is limiting the heating and loss of atoms from the trap due to collisions with the background gas and other metastable atoms. The dominant loss process in metastable neon traps is ionization.
1.5.1 Loss

The large electronic energy of \( \text{Ne}^* \) \( ^3P_2 \) of 16.6 eV, is always enough to allow for ionization in binary collisions. The process of ionization of metastable neon atoms \( \text{Ne}^* \) in the \( ^3P_2 \) state is given by [3]:

\[
\text{Ne}^* (^3P_2) | J = 2, m_J \rangle + \text{Ne}^* (^3P_2) | J = 2, m'_J \rangle \rightarrow \text{Ne}(^1S_0) + \text{Ne}^+ + e^- \quad \text{PI}
\]

\[
\rightarrow \text{Ne}_2^+(v) + e^- \quad \text{AI}. \tag{1.6}
\]

Here \( J \) is the total angular momentum quantum number and \( m_J \) the projection of the total angular momentum on the axis of quantization, indicating the magnetic substate.

Ionization is based on the exchange mechanism between the electrons involved, due to their Coulomb interaction. When two \( \text{Ne}^* \) atoms collide, a valence electron of one of the \( \text{Ne}^* \) atoms (1) fills up the hole in the \((2p^5)\) core of the other \( \text{Ne}^* \) atom (2). The valence electron in the \( 3s \) state of the latter atom (2) is no longer bound and escapes. Its kinetic energy is of the order of 12 eV. In the case of Penning ionization (PI) (1.6), the former atom (1) consists now only of a positive core. In the case of Associative ionization (AI) (1.6), both the resulting atoms form a molecular ion.

The resulting ground state \( \text{Ne} \) ions and atoms carry each an energy in the range 100 – 500 K, depending on the energy gained in the well of the initial state potential and the internuclear distance where ionization occurs. The probability for ionization is maximum at the turning points of the initial state potential, where the atoms spend most of their time.

Associative Ionization only occurs when the two metastable \( \text{Ne}^* \) atoms decay around the inner turning point of the initial state potential and decay to a bound state. However, chances are very small that the two metastable \( \text{Ne}^* \) atoms will reach this spot. Therefore the branching ratio for Associative Ionization is very small, on the order of 0.01 – 0.1. Almost all initial kinetic energy is stored in the molecular ion as vibrational energy. Only the recoil energy of the electron kick is important for estimating the heating rate.

**Suppression of Ionization**

In fully stretched (polarized) states, such as the \( ^3P_2, m_J = 2 \) and the \( ^3D_3, m_J = 3 \) state, the available electron state in the core has the opposite spin from the valence electron. As a consequence, the spin of the valence electron needs to flip in order to be able to fill up the hole in the core of the other \( \text{Ne}^* \) atom. In Penning ionization this spin flip is, however, in first order approximation forbidden. Spin flipping, and thus ionization, then only occurs through weaker processes such as spin-dipole and spin-orbit interaction, resulting in only a small probability for ionization. The long-range quadrupole-quadrupole interaction due to the \((2p)^{-1}\) core holes will cause a torque that can rotate the total angular momentum \( J \) of the atoms involved with respect to each other. This will result in residual ionization and thus loss and/or heating [23]. However, the ionization rate will be strongly suppressed for these polarized atoms.

Detailed quantum mechanical calculations of the ionization rates for cold collisions performed by Doery et al. [23] yield the following ionization rate constants for the unpolarized, \( \kappa_{\text{ion}} \), and polarized (doubly stretched) \( \kappa_{\text{ion}}^{\text{pol}} \) case, respectively:

\[
\kappa_{\text{ion}} = 5 \times 10^{-11} \text{cm}^2 \text{s}^{-1} \\
\kappa_{\text{ion}}^{\text{pol}} \leq 5 \times 10^{-15} \text{cm}^2 \text{s}^{-1}. \tag{1.7}
\]
1.5.2 Heating

Ionizing collisions of metastable rare gas atoms directly result in the loss of trapped atoms because the final state products (the so-called hot products) are magnetically untrapable and will have large kinetic energies, which enables them to escape from the trap. The resulting hot products can also collide with cold trapped atoms and transfer some of their kinetic energy on their way out of the trap. Extra loss and heating of atoms from the trap is the result, especially when the mean free path of the hot products in the trap is sufficiently small. The mean free path is the average distance which an atom travels before it scatters off or collides with another atom.

Heating also occurs when the transferred energy $\Delta E$ in collisions with hot, background atoms is less or of the same order as the trap depth $\Delta E \leq \mathcal{E}$. The heated atoms do not leave the trap but dissipate their excess energy in collisions with other trapped atoms. As a consequence, the average temperature of the atoms in the trap will increase, which could be fatal for reaching or maintaining a BEC. A finite trap depth $\mathcal{E}$ results in an upper bound for the energy transfer that will still result in heating. Lowering the trap depth will, however, not only reduce the heating effect, but will also reduce the number of particles in the trap. Characteristic values for the trap depth are $1\text{ - }5 \text{ mK}$.

Four collisional processes result in heating and/or loss of trapped atoms: collisions with the background gas, ionizing collisions, ion-metastable atom collisions and atom-metastable atom collisions. In addition, heating by UV-photon recoils must be taken into account.

An extensive treatment of heating in metastable neon traps by Beijerinck [3] shows that the main contribution to the heating rate is supplied by ion-metastable atom collisions. He also shows that heating is less in a cigar-shaped trap with a large aspect ratio. The aspect-ratio is defined as the ratio of the long to the small axis of an ellipse or the ratio of the radial trapping frequency, $\omega_r$, and the axial trapping frequency $\omega_z$ and is equal to $\omega_r/\omega_z$. The average distance the atoms travel in the trap is strongly reduced, since the atoms have a large probability of leaving the trap along the short axis. Therefore, we use in our experiments a cigar-shaped trap.

1.6 This report

This report consists of three main parts. In chapter 2 the magnetic fields of the MOT, and in particular the MT, are discussed in detail, since the realization of a BEC depends critically on whether certain trapping conditions are met or not.

Second, in chapter 3, the condition for the MOT are discussed. First measurements on the number of trapped particles in the MOT, the particle density and the loss rate constant due to ionization, are presented.

Third, in chapter 4, calculations on the photo-association process are presented. Since very little is known about the interaction potentials of metastable neon, future measurements entail, among other things, photo-association spectroscopy (PAS). Photo-association spectroscopy is a powerful technique to obtain, in combination with calculations, information on the interaction potentials of metastable neon. Moreover, the scattering length of neon can be determined from comparing PAS-measurements with the calculations. To conclude, concluding remarks and recommendations are given in chapter 5.
1.7 Units

Throughout this report, we will denote the particle density $n$ and the volume $V$ in units of $\text{cm}^{-3}$ and $\text{cm}^3$, respectively. The strength, gradient and curvature of magnetic fields are expressed in $\text{G}$, $\text{G/mm}$ and $\text{G/mm}^2$, respectively.
Chapter 2

Magnetic fields in atom traps

2.1 Introduction

To realize BEC we load a cold bright beam of metastable neon atoms in a MOT and successively cool them to temperatures below the BEC transition temperature $T_C$. In order to achieve BEC, stringent requirements on the trapping fields must be met. In this chapter these requirements are discussed and is investigated whether our magnetic trap fits these criteria.

2.1.1 Transfer from MOT to MT

The magnetic trap is loaded from the MOT. In order to minimize loss of phase space density during the transfer both traps should overlap and the potential of the MT must meet certain requirements.

The potential of the MOT can be represented by a three-dimensional box potential:

$$U_{MOT}(x,y,z) = \begin{cases} 0 & \text{if } -l/2 < x_i < l/2, \\ \infty & \text{otherwise}, \end{cases}$$

(2.1)

where $x_i$ is either $x$, $y$ or $z$ and $l$ is the trap dimension, so that the volume of the MOT is equal to $V = l^3/2$. The size $l_z = l/2$ of the trap in the axial direction is half the size $l_x = l_y = l$ of the trap in the $x$- and $y$- direction, (aspect ratio 0.5). The potential of the MT is approximated by a cylindrically symmetric, harmonic potential:

$$U_{MT}(x,y,z) = \frac{m}{2} \left( \omega_r^2 x^2 + y^2 + \omega_z^2 z^2 \right),$$

(2.2)

where $\omega_r$ and $\omega_z$ are the radial and axial trapping frequency, respectively, and $m$ the atomic mass.

The transfer from MOT to MT is modeled as a sudden change in the potential. The box potential of the MOT is instantaneously replaced by the harmonic potential of the MT. The centers of both potentials coincide. The loss of phase space density during the transfer from the MOT to the MT is minimum if the ratio of the phase space density in the MT to that in the MOT, is maximum. This condition yields the optimum trapping frequencies of the trapping potential of the MT [34]:

$$\omega_r = \frac{1}{2} \omega_z = \left( \frac{12kBT}{ml^2} \right)^{1/2}.$$  

(2.3)
Magnetic fields in atom traps

It can easily be shown that, for an optimum transfer of atoms, the equilibrium temperatures in both traps must be equal. For an optimum temperature of $40 \mu$K in the MOT and a minimum MOT dimension of $l = 5.8 \text{ mm}$ (in chapter 3 we will see that the minimum dimension of our MOT is $l = 5.8 \text{ mm}$) the optimum trapping frequencies are $\omega_r = \omega_z / 2 = 12.3(2\pi) \text{ Hz}$. However, this radial trapping frequency is experimentally not feasible. The maximum possible axial trapping frequency is $\omega_z = 48(2\pi) \text{ Hz}$. For this trapping frequency, the minimum radial trapping frequency achievable is $\omega_r = 47(2\pi) \text{ Hz}$.

Special cooling techniques (sub-Doppler cooling) must be applied to obtain a MOT temperature of $40 \mu$K. A typical temperature achievable when using only Doppler laser cooling is $\approx 200 \mu$K. Assuming the same MOT dimension, the optimum trapping frequencies are then $\omega_r = \omega_z / 2 = 27.4(2\pi) \text{ Hz}$. The optimum axial trapping frequency lies now close to the experimental limit. The optimum radial trapping frequency is, however, still much lower than the experimental limit. As a result, loss of phase space density after the transfer from MOT to MT is not minimum. when using the best solution experimentally feasible $\omega_r = \omega_z = 48(2\pi) \text{ Hz}$, a factor of 1.7 in phase space density is lost as compared to the optimum case. However, since the phase space density needs to be increased by a factor of $10^5$ in the MT to obtain the critical BEC phase space density, this is not a problem. Cooling the atoms to $40 \mu$K, instead of $200 \mu$K, in the MOT will increase the loss in phase space density during the transfer from MOT to MT with a factor 5. Since the absolute phase density increases with a factor $11 (D \propto T^{-3/2}(1.1))$, cooling the atoms in the MOT to $40 \mu$K will yield a gain in phase space density of a factor 2, after transferring the atoms from the MOT to the MT.

Summarizing, the first requirement the MT must meet is that it should have a weak harmonic trapping potential, to minimize the loss of atoms and phase space density during the transfer from MOT to MT.

2.1.2 Adiabatic compression and evaporative cooling

After loading the MT, the trapping potential of the MT is adiabatically ramped up, resulting in a tight radial confinement, to increase the phase space density and reduce the heating due to ion-metastable atom collisions [4]. Here adiabatic means that, if a particle was originally in the $n$th eigenstate of the trapping potential, after transferring the particles from the MOT to the MT and increasing the magnetic field gradient, it will also be in the $n$th eigenstate of the new trapping potential.

The transition temperature $T_c$ for Bose-Einstein Condensation is defined as the temperature for which in the ground state a single macroscopic quantum state is formed. For a harmonic trap the transition temperature is given by [34]:

$$k_B T_c = \hbar \left( \frac{N \omega_x \omega_y \omega_z}{2} \right)^{1/3} \approx 0.94 \hbar N^{1/3} \omega_z^{2/3} \omega_x^{1/3}. \quad (2.4)$$

Beijerinck [4] showed that in a trap with a large aspect ratio heating is reduced (1.5.2). The maximum radial trapping frequency achievable in our setup is $\omega_r = 480(2\pi) \text{ Hz}$. For a trap with aspect-ratio $\omega_r / \omega_z = 10$, during the adiabatic compression phase, and containing $N = 10^6$ atoms (a characteristic value of the number of ultra cold atoms that are still trapped after the transfer from MOT to MT and evaporative cooling), the transition temperature for achieving BEC (2.4) is equal to $T_C = 1 \mu$K.

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So, the second requirement the MT must meet is that it should have a tightly confining potential, after the adiabatic compression phase, to cool the atoms below the critical BEC transition temperature. Since, on the other hand, a weak harmonic trapping field yields a minimum loss of phase space density during the transfer from the MOT to the MT, the magnetic field produced by the MT must be tunable.

2.1.3 Trapping conditions

To minimize trap losses by ionization (see § 1.5.2) the trap depth should be limited and the aspect-ratio of the trap geometry should be large. The experimentally maximum aspect-ratio we can achieve is $\omega_r/\omega_z = 10$. For heating effects to be limited to acceptable values, the trap depth must be 10 mK at the maximum [3]. This leads to a condition for the maximum magnetic field strength difference or magnetic field depth [34]: $\Delta |\vec{B}| \leq k_B T/\mu = 50 \text{ G}$, where $\mu$ is the magnetic moment of the atom.

In addition, loss of atoms from the trap during the transfer from the MOT to the MT should be minimized. Therefore, the depth of the magnetic trap must be sufficiently large so that not only all atoms are transferred from the MOT to the MT, but also all atoms remain confined during the adiabatic compression. In order to transfer as many atoms as possible from the MOT to the MT, the depth $\Delta |U|$ of the potential of the MT must be larger than the average total energy $E_T$ of each atom. This leads to a field depth of [34]: $\Delta |\vec{B}| = \Delta |U|/\mu \geq 50 \text{ G}$. Stas [34] also showed that in order to confine (almost) all atoms during the adiabatic compression, the minimum field depth equals $\Delta |\vec{B}| \geq 36 \text{ G}$. Compromising between all these conditions yields:

$$\Delta |\vec{B}| \approx 50 \text{ G}. \quad (2.5)$$

In addition, an in-homogeneous magnetic field with a local field minimum is necessary to trap the atoms in the first place. When the minimum of this trapping magnetic field is equal to zero, however, the confined atom can make Majorana (spin flip) transitions to non-trapped states, see § 1.4.2, and atoms will be lost from the trap. For an efficient tight confinement on the other hand, the minimum value of the bias magnetic field should be as low as possible. Together these conditions yield for the minimum magnetic field strength:

$$B_0 \approx 1 \text{ G}. \quad (2.6)$$

2.1.4 This chapter

We have seen that certain trapping requirements need to be met in order to achieve Bose-Einstein condensation. Therefore we will look in this chapter in more detail at the trapping magnetic fields of both the MOT and MT. Especially the trapping fields of our MT, the Clover Leaf trap, are discussed in detail. A Clover Leaf trap was chosen because it provides the required harmonic trapping potential which satisfies the trapping requirements discussed above.

This chapter is organized as follows: first the magnetic fields of the Clover Leaf trap are described. Second, both the design of the MOT and the Clover Leaf trap, which are based on calculations of the bias magnetic field and the magnetic field gradient and curvature, are described in § 2.3. In § 2.4 these calculations are presented. Next, measurements of the magnetic fields are discussed in § 2.5, in order to determine whether our design fits the trapping criteria. These measurements showed that the design had to be slightly altered to fit the trapping criteria. In addition, the coils had to be protected against overheating and thus had to be taken apart. The relative position of the coils with
2.2. THE CLOVER LEAF TRAP

The Clover Leaf trap consists of two Bias, two Pinch and eight Gradient coils as shown in Figure 2.1. The axis perpendicular to the coils is the z-axis. The direction of the current through the coils is given. The Bias coils generate an axial bias magnetic field $B_{0,b}$ along the z-axis. The Pinch coils generate an opposing axial magnetic field consisting of a constant homogeneous bias magnetic field $B_{0,p}$ and a non-homogeneous magnetic field with curvature $B'' = \frac{\partial^2 B}{\partial z^2}$, which provides the axial confinement. The total axial magnetic field generated by the Bias and Pinch coils is, at small $z$, equal to:

$$ B_t = B_{0,t} + \frac{1}{2} B'' z^2, \quad (2.7) $$

where the total axial bias magnetic field is given by: $B_{0,t} = B_{0,b} + B_{0,p}$. Figure 2.2a shows the magnetic fields generated by the Bias and Pinch coils.

The Gradient coils generate a radial magnetic quadrupole field with gradient $B' = \frac{\partial B}{\partial r}$, which provides the radial confinement. The total magnetic field strength $|\vec{B}|$, consisting of the axial and radial magnetic fields, is harmonic near $r = 0$ and linear at larger distances. Figure 2.2b shows two curves of the total magnetic field strength. The upper curve is the weak axial trapping field with a large total bias magnetic field, required to transfer the atoms from the MOT to the MT with a minimum loss of phase space density. The lower curve is the total axial magnetic field with a small total bias magnetic field, required to compress and cool the atoms to temperatures below the BEC transition temperature.
Magnetic fields in atom traps

Figure 2.2: Axial magnetic fields of, a, the Bias and Pinch coils as a function of z and, b, the absolute value of the total magnetic field \( |\vec{B}(r)| = \sqrt{(B_t^2 + B_r^2)} \) of the Clover Leaf trap as a function of r. Here \( B_t \) is the total axial magnetic field of the Bias and Pinch coils and \( B_r \) the radial magnetic quadrupole field of the Gradient coils. The figure clearly shows that the magnetic field strength \( |\vec{B}| \) is harmonic near the center of the trap \( r = 0 \), and linear at larger distances. Curves of the total field strength \( |\vec{B}| \) are drawn for a weak trapping potential (loading), and a tightly confining trapping potential (compression). The former is necessary to transfer the atoms from the MOT to the MT with a minimum loss of phase space density, the latter is necessary to compress the atoms during the evaporative cooling phase. The weak trapping potential (loading) has a large axial bias magnetic field \( B_{0,l} \sim 100 \) G. The tightly confining potential (compression) has a very small (positive) axial bias magnetic field \( B_{0,c} \sim 1 \) G.
2.3. DESIGN OF THE TRAPS

In the design of the Clover Leaf trap are also two additional Fine tuning coils incorporated (not shown in Figure 2.1). These can be used to make small adjustments in the total axial bias magnetic field of the Bias and Pinch coils, to make sure that this field is positive and of the order of 1 G (§ 2.1.3). The Fine tuning coils are wrapped around the Pinch coils.

2.3 Design of the traps

Both the Bias and Pinch coils have been designed by Stas [34] in such a way that, when the current through both coils equals 200 A, the total axial bias magnetic field at the center of the trap \((r = 0)\) is of the order of 1 G (§ 2.1.3). Because this total bias magnetic field is so small, it is very important that the magnetic fields of the Bias and Pinch coils are very stable. Therefore, the Bias and Pinch coils are connected in series. The current through the Bias coils can be tuned to generate (in combination with the Pinch coils) a large total (positive) axial bias magnetic field during the transfer from the MOT to the MT and a small total axial bias magnetic field during the compression and cooling phase, using a switchable electronic shunt.

Figure 2.3 shows two cross sections of the coil configuration of the Clover Leaf trap and MOT. Figure 2.3a gives a schematic view of the Gradient coils perpendicular to the \(z\)-axis. Figure 2.3b shows a cross section of the coil configuration in the \(y, z\)-plane. The coils consist of multiple layers, \(N_l\), along the \(z\)-axis, each of which contain \(T_{pl}\) turns, along the \(r\)-axis. Table 2.1 gives the experimental parameters of the coils.

The MOT coils are made of hollow round copper tube with an inner diameter of 2.0 and an outer
2.4. **Calculation of the Magnetic Fields**

### Table 2.1: Geometry of the coils

<table>
<thead>
<tr>
<th>Coils</th>
<th>Turns</th>
<th>Tpl</th>
<th>Nl</th>
<th>R (mm)</th>
<th>A (mm)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Bias</td>
<td>17</td>
<td>4 a</td>
<td>4</td>
<td>80</td>
<td>60</td>
</tr>
<tr>
<td>Pinch</td>
<td>12</td>
<td>4</td>
<td>3</td>
<td>16</td>
<td>30</td>
</tr>
<tr>
<td>Fine tuning</td>
<td>6</td>
<td>2</td>
<td>3</td>
<td>31</td>
<td>30</td>
</tr>
<tr>
<td>Gradient</td>
<td>20</td>
<td>5</td>
<td>4</td>
<td>20-80 b</td>
<td>45</td>
</tr>
<tr>
<td>MOT</td>
<td>24</td>
<td>8</td>
<td>3</td>
<td>43</td>
<td>60</td>
</tr>
</tbody>
</table>

*a* The Bias coil consists of 17 turns: 4 layers of 4 turns + 1 turn extra in the first layer (Figure 2.3 b).

*b* The inner radius of the gradient coils, approximated by a quarter of a circle, is 20 and the outer radius equals 80 mm.

*c* Uncertainty is ±1 mm.

The coils of the Magnetostatic Trap are made of hollow square copper tubing. The outer dimension of these tubes is 3.2 mm and they have a thickness of 0.8 mm. The total outer dimension of the tubes, including the fibreglass insulation equals 3.6 mm.

The tubes are hollow because they need to be cooled with water, since a lot of heat is dissipated with currents of \( I \approx 200 - 300 \) A, which are necessary in order to meet the trapping requirements. The increase in surface temperature of the Gradient coils as a function of the current \( I \) through the coil is given in Appendix B.

The coils of the MOT and Clover Leaf trap are placed around a stainless steel vacuum chamber according to Stas' [34] design. Part of the construction drawing is shown in Figure 2.4. The stainless steel chamber has windows on all sides. The larger side windows are positioned inwards and have a diameter of 80 mm. The Pinch and Fine tuning coils are fit into the free space in front of these windows. Comparing Figure 2.3 and 2.4, it is clear that the coils of the Clover Leaf trap and the MOT fit exactly around the trapping chamber.

#### 2.4.1 Analytical description of the magnetic fields

The total combined magnetic field of the Bias, Pinch and Gradient coils is in good approximation given by [34]:

\[
\text{Total Magnetic Field} = \text{Bias Field} + \text{Pinch Field} + \text{Gradient Field}
\]
Figure 2.4: Part of the construction drawing of the vacuum chamber. The cross section, a, through the $xy-$plane and the cross section, b, through the $xz-$plane. Cross section a shows the trapping chamber with 4 windows under an angle of $\pm 45^\circ$ with respect to the $x-$ and $y-$axis. The broad arrows indicate the light beams of the MOT and the Zeeman slower beam. The left window along the horizontal $y-$axis is used for the extra Zeeman slower beam and the atoms enter the chamber through the port on the right. To the upper port along the vertical $x-$axis a channeltron is attached (§ 3.4.2). To the lower port along the $x-$axis a CCD camera is attached. The two windows in the center of the chamber transmit the horizontal, orthogonal set of counter propagating MOT beams, as shown in the second cross section b.
Table 2.2: Calculated values of the total bias magnetic field $B_{0,t}$, the magnetic field gradient $B'$ and the magnetic field curvature $B''$ for all coils of the Clover Leaf trap combined, and the current $I$ through each coil. These values are calculated using equations (A.4), (A.5) and (2.9). Applying a magnetic trapping field satisfying these requirements yields an optimum transfer of phase space density and optimum evaporative cooling conditions achievable.

<table>
<thead>
<tr>
<th>Coil</th>
<th>$I \pm 0.1$ (A)</th>
<th>magnetic field parameters</th>
<th>$I \pm 0.1$ (A)</th>
<th>magnetic field parameters</th>
</tr>
</thead>
<tbody>
<tr>
<td>Bias</td>
<td>117</td>
<td>$B_{0,t} = 99.6$ G</td>
<td>200</td>
<td>$B_{0,t} = 1.5$ G</td>
</tr>
<tr>
<td>Pinch</td>
<td>200</td>
<td>$B'' = 1.1$ G/mm$^2$</td>
<td>200</td>
<td>$B'' = 1.1$ G/mm$^2$</td>
</tr>
<tr>
<td>Gradient</td>
<td>300</td>
<td>$B' = 12.7$ G/mm</td>
<td>300</td>
<td>$B' = 12.7$ G/mm</td>
</tr>
</tbody>
</table>

\[ B_r = B'r \sin 2\phi - \frac{1}{2}B''rz + \cdots, \]
\[ B_\phi = B'r \cos 2\phi + \cdots, \]
\[ B_z = B_0 + \frac{1}{2}B''(z^2 - \frac{r^2}{2}) + \cdots, \]
\[ |\vec{B}| = \left[(B_0 + \frac{1}{2}B''z^2 + r^2(B'^2 - \frac{1}{2}B_0B'') + \cdots\right]^{1/2}. \]

In Appendix 5 the approximations made are explained and simple analytical expressions for the magnetic fields of each of the Clover Leaf coils and the MOT coils are given. The magnetic field gradient $B'$ and the magnetic field curvature $B''$ are defined in equation (A.4) and (A.5), respectively.

From equation (2.8) it is clear that $|\vec{B}(\vec{r} = \vec{0})| = |B_0|$. This axial field is generated by the Bias and Pinch coils. The total magnetic field is a combination of a radial quadrupole field, due to the Gradient coils, and a harmonic axial field, due to the Bias and Pinch coils. The total magnetic field is harmonic near the center of the trap for $r < B_0/B'$ and linear at larger distances (Figure 2.2).

In the former range the trapping potential $U$ is harmonic and cylindrically symmetric. Comparing equation (2.2) and (2.8) we find the relation between the trapping frequencies and the magnetic field parameters of the Clover Leaf trap:

\[ U(\vec{r}) = U_0 + \frac{m}{2}(\omega_z^2z^2 + \omega_r^2r^2), \]
\[ U_0 = \mu B_0, \]
\[ \omega_z = (\mu B''/m)^{1/2}, \]
\[ \omega_r = \left[\frac{\mu}{m}(B'^2/B_0 - B''/2)\right]^{1/2}, \]

where $\mu$ is the magnetic moment of the atom, $m$ the atomic mass and $U_0$ the minimum potential energy. Table 2.2 gives the trapping frequencies and the magnetic field parameters for the transfer from the MOT to the MT and for the evaporative cooling stage.

The MOT coils generate a spherical quadrupole magnetic field which increases to first order linearly with the spatial coordinates (§ A.7).
Table 2.3: The calculated values of the axial bias magnetic fields $B_0$, the magnetic field gradient $B'$ and the magnetic field curvature $B''$ for each coil at $(x, y, z) = (0, 0, 0)$. All values are calculated using Stas' Maple program [34]. The axial magnetic field of the Bias coils is calculated for respectively 17 and 15 turns. The axial bias magnetic fields are calculated for $I = 200 \, \text{A}$ and the radial gradient quadrupole field is calculated for $I = 300 \, \text{A}$, because then the calculated values of the axial magnetic field curvature $B''$, and the radial magnetic field gradient, $B'$, are of the order of magnitude of the trapping conditions and yield the best (possible) trapping frequencies, see Table 2.2.

<table>
<thead>
<tr>
<th>Coil</th>
<th>Turns</th>
<th>$I$(A)</th>
<th>$B_0$ (G)</th>
<th>$B'$ (G/mm)</th>
<th>$B''$ (G/mm²)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Bias</td>
<td>17 $^a$</td>
<td>200</td>
<td>-254</td>
<td>-</td>
<td>-0.054</td>
</tr>
<tr>
<td>Bias</td>
<td>15</td>
<td>200</td>
<td>-222</td>
<td>-</td>
<td>-0.050</td>
</tr>
<tr>
<td>Pinch</td>
<td>12</td>
<td>200</td>
<td>229</td>
<td>-</td>
<td>1.06</td>
</tr>
<tr>
<td>Fine tuning</td>
<td>6</td>
<td>5.0</td>
<td>4</td>
<td>-</td>
<td>0.0084</td>
</tr>
<tr>
<td>Gradient</td>
<td>20</td>
<td>300</td>
<td>-</td>
<td>12.73</td>
<td>-</td>
</tr>
<tr>
<td>MOT</td>
<td>24</td>
<td>26</td>
<td>-</td>
<td>1.0</td>
<td>-</td>
</tr>
</tbody>
</table>

$^a$The number of turns in the original design

2.4.2 Numerical calculations

Table 2.3 gives the numerical values of the bias magnetic field $B_0$, the magnetic field gradient $B'$, and the magnetic field curvature $B''$, for all the coils of the Clover Leaf trap and MOT at $r = 0$. These values have been calculated with Stas' Maple program [34], using the coil parameters given in Table 2.1.

The uncertainty in either $R$ or $A$ is ±1 mm. This uncertainty has a much larger effect on the magnetic field of the Pinch coils than on the magnetic field of the Bias coils, since both the radius $R$ and the distance between the coils $2A$ are much smaller for the Pinch than for the Bias coils. The estimated total uncertainty in the axial bias magnetic field, due to an uncertainty of 1 mm in both $R$ and $A$, is, respectively, 2 % and 16 %, for the Bias and the Pinch coils at the center of the trap and $I = 200 \, \text{A}$. The total uncertainty in the curvature of the axial bias magnetic field is, respectively, 25 % and 33 %, for the Bias and the Pinch coils at the center of the trap. The total uncertainty in the axial MOT magnetic field gradient, due to an uncertainty of 1 mm in both $R$ and $A$, is equal to 6 % at the center of the trap and $I = 30 \, \text{A}$.

From Table 2.3 we obtain the values of the total axial bias magnetic field, $B_{0,t}$, of the Pinch and Bias coils combined for, respectively a Bias coil consisting of $N_b = 17$ and $N_b = 15$ turns:

\[
\begin{align*}
B_{0,b} + B_{0,p} &= -25.03 \, \text{G} \quad N_b = 17, \\
B_{0,b} + B_{0,p} &= +6.39 \, \text{G} \quad N_b = 15.
\end{align*}
\]

(2.10)

These values clearly show that a Bias coil consisting of 17 turns generates too strong a negative magnetic field; the total bias field is negative, which causes trap losses (§ 2.1.3). However, when two turns are removed ($N_b = 15$), the resulting axial bias magnetic field is positive.

Removing 2.5 turns would yield an even better result for the total axial bias magnetic field. However, due to the loss of symmetry of the resulting coil configuration, the transverse magnetic
field will not cancel out anymore. The result is not only the desired axial magnetic field, but also a transverse magnetic field of the order of $|B_{0,\perp}| \approx 8 \text{ G}$. This is an order of magnitude more than the desired total axial bias field of $|B_{0,\parallel}| \approx 1 \text{ G}$. Clearly it is not an option to remove only part of a turn.

2.5 Magnetic field measurements

2.5.1 Experimental setup

The magnetic fields of the different coils have been measured using a three dimensional probe, consisting of three LohetII Hall probes with a sensitivity of $25 \pm 0.5 \text{ mV/G}$ aligned along the cartesian coordinate axes. A schematic view of the geometry of the experimental setup, including the definition of the axes in this system, is given in Figure 2.5. Also the direction of the current through the loops is indicated for the Bias, Pinch, Gradient and MOT coils. To measure the magnetic fields of the MT and the MOT, the stainless steel chamber is temporarily replaced by a wooden dummy chamber with holes in it. A picture of the experimental setup is shown in Figure 2.6.

The output voltage of the Hall probe [13] varies in proportion to the strength of the external magnetic field. The measurement range of the probe is $-100$ to $+100 \text{ G}$. The probe operates from an 8 V dc supply, and at its maximum range the output voltage will be typically $\approx 6.5 \text{ V}$. The output voltage at 0 G is typically 4.0 V. For the earth magnetic field offset has been corrected.

The magnetic field measurements presented in subsections 2.5.3, 2.5.4 and 2.5.5 were taken at a current of $I = 10 \text{ A}$ through the coils because the watercooling had not been installed yet. Without watercooling the coils would heat up dramatically for currents of the order of 200 A. As a consequence the measured magnetic fields are rather small. Therefore, the signal of the probes is first amplified 10
times before it is read by a 12-bit dual mode Analog to Digital Converter (ADC) [31] and converted to its corresponding magnetic field value. The uncertainty in this 10 times amplified signal, due to a remaining slight offset, is equal to $\approx 2 \text{ mV} = 0.08 \text{ G}$ and is corrected in the analysis of the measurements. The sensitivity of the probe introduces an uncertainty of 2% in the measurements. The signal of the ADC is read out a hundred times and averaged for each measurement. The minimum change in the magnetic field, which the ADC can measure, is 0.2 mV corresponding to 0.008 G for the 10 times amplified signal.

The spatial dependence of the magnetic field has been measured in three dimensions by mounting the three probes on a three-dimensional manipulator, controlled by an eight Channel Stepper Motor Controller [32] incorporated in a Phyas interface. The resolution of the Stepper Motor is 0.0025 mm for the $y$- and $z$-axis and 0.01 mm for the $x$-axis. The measurements are operated/controlled by an EPEP [11] program.

The geometrical center of the trap is determined using a telescope along two coordinate axes. The holes in the dummy wooden chamber are used as a reference. For each measurement the center of the relevant probe coincides with the geometrical center of the trap.

The uncertainty in determining the exact location of the geometrical center of the trap is difficult to assess. First, the holes in the dummy, wooden chamber are not perfectly aligned and as a consequence neither is the telescope. The misalignment is estimated at $< 2 \text{ mm}$. This introduces an error of $< 1 \text{ mm}$ in the spatial coordinates. In addition, the exact center of the Hall probe is difficult to determine. Together this might introduce an uncertainty of $< 1.5 \text{ mm}$ in the determination of spatial coordinates of the center of the trap. An error due to a possible slight misalignment of the coordinate-axes of the manipulator and the Clover Leaf trap, is negligibly small in comparison.
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Figure 2.7: The axial Bias magnetic field as a function of $z$ measured with probe I and II at $(x, y) = (0, 0)$ mm and $I = 75$ A. Both graphs are fitted with $B_z = B_{0,z} + \frac{1}{2} B''_z (z - z_0)^2$.

Table 2.4: Measured values of the bias magnetic field $B_0$ and the magnetic field curvature $B''$ per Ampère for the Bias coils in the final coil configuration at $(x, y) = (0, 0)$ mm and $I = 75$ A. Both $B_0$ and $B''$ are obtained from fitting the measurement data with equation (2.11). The axial Bias magnetic field is measured with both probe I and II.

<table>
<thead>
<tr>
<th>Probe</th>
<th>Range (G)</th>
<th>Sensitivity (mV/G)</th>
<th>$B_{0,z}$ (G/A)</th>
<th>$B''_z$ (G/A mm$^2$)</th>
<th>$z_0 \pm 1.5$ (mm)</th>
</tr>
</thead>
<tbody>
<tr>
<td>I</td>
<td>$\pm 100$</td>
<td>$25.0 \pm 0.5$</td>
<td>0.93</td>
<td>0.00026</td>
<td>2.2</td>
</tr>
<tr>
<td>II</td>
<td>$\pm 2500$</td>
<td>$1.00 \pm 0.02$</td>
<td>0.97</td>
<td>0.00024</td>
<td>1.8</td>
</tr>
</tbody>
</table>
Figure 2.8: Axial Bias magnetic field as a function of $z$ for $(x,y) = (0,0)$ and $I = 75$ A. The experimental data are fitted with $B_z = B_{0,z} + \frac{1}{2}B''_z(z - z_0)^2$

2.5.2 Probe calibration

The Hall probe with a measurement range of $-100$ to $100$ G (probe I), which has been used to measure the magnetic fields, is calibrated with another calibrated Hall probe with a range of $-2500$ to $2500$ G (probe II). The latter Hall probe (probe II) was first calibrated with a gauge magnet $^1$ of $100 \pm 1$ G. Measuring the magnetic field of the gauge magnet with Probe II yields a value of $99$ G, so probe II is well calibrated.

Then both probes are compared using the axial bias magnetic field of the Bias coils at $I=75$ A. The results are given in Table 2.4 and Figure 2.7. We conclude that the measured values of the axial bias magnetic field $B_{0,z}$ agree within $4\%$ and the measured values of the axial magnetic field curvature $B''_z$ within $5\%$. Or in other words, probe I is accurate within its sensitivity of $2\%$.

2.5.3 Axial magnetic field

Figure 2.8 shows the axial magnetic field of the Bias coils. It clearly shows that the magnetic field is in good approximation parabolic as a function of $z$. The curvature of the magnetic field is, however, small in comparison to the curvature of the Pinch coils. The values of the axial bias magnetic field $B_0$, the curvature $B''_z$ of the magnetic field and the displacement $d_0 = z_0$ of the minimum of the magnetic field are given in Table 2.5. Both $B_0$, $B''_z$ and $z_0$ are obtained from fitting the experimental data with:

$$B_z = B_{0,z} + \frac{1}{2}B''_z(z - z_0)^2.$$  \hspace{1cm} (2.11)

The axial magnetic Bias field is approximately constant (very small curvature) and equals: $B_{0,b} =$

---

$^1$D343-1000 Gap .343 gauge magnet of RFL industries Inc. Boonton, New Jersey, USA

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1.16 G/A (Table 2.5). Also the x- and y-components of the Bias magnetic field are constant and approximately zero in all directions.

Figure 2.9 shows the axial Pinch magnetic field $B_z$ as a function of $z$ for different $x$-coordinates and $y = 0$. The parabolic nature of the axial Pinch magnetic field as a function of $z$ is clearly visible. The picture also clearly shows a saddle point in the Pinch magnetic field at about $x = 1$ mm.

The bias Pinch magnetic field $B_{0,p}$ is about 1.02 G/A at its maximum and about 0.86 G/A at its minimum value. The Pinch magnetic field curvature ranges from $B'' = 0.0042$ G/Am$^2$ to $B'' = 0.005$ G/Am$^2$, for the different curves as a function of $x$. The magnetic field is minimum at $z_0 = (1.4 \pm 0.2)$ mm.

Figure 2.10 shows the measured combined Bias and Pinch axial magnetic field as a function of the $z$-coordinate. Again the field is parabolic, as expected. The figure also clearly shows that the total bias magnetic field of the Bias (consisting of 17 turns) and Pinch coils combined is negative, which leads to trap losses, see §1.4.2. Therefore, a compensating Fine tuning field should be applied.

From Figure 2.10 and Table 2.5 (measured values) we obtain a total axial bias magnetic field of the Bias and Pinch coils combined equal to:

$$B_t(z) = -26.6[G] + 0.46[G/mm^2] \times (z + 1.2)^2[mm^2],$$

(2.12)
at $I = 200$ A. This is in agreement with the calculations (§ 2.4). At $I_b = I_p = 200$ A, a (calculated) current of $I_I = 42$ A through the Fine tuning coils is necessary to achieve a total bias magnetic field of $\approx 1$ G at the center of the trap. The Fine tuning coils have been designed, however, for much lower currents. Therefore, this measurement confirms the necessity for removing some turns from the Bias coils (§ 2.3).

Comparing the calculated and measured values of the magnetic fields in Table 2.5, it immediately becomes clear that the measured values are consistently lower than the calculated values. The axial
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Figure 2.10: Sum of the axial Pinch and Bias magnetic field as a function of \( z \) at \( I_b = I_p = 10 \) A and \( (x, y) = (0, 0) \), where \( I_b \) and \( I_p \) are, respectively, the current through the Bias and Pinch coils. The Bias coils consist of 17 turns each. The magnetic field is fitted using equation (2.11).

Table 2.5: Measured and calculated values of the bias magnetic field \( B_0 \), the magnetic field gradient \( B' \), and the magnetic field curvature \( B'' \) per Ampère for each coil. All parameters are obtained from fitting the experimental data with either equation (2.11) or (2.13). For the Bias, Pinch, Fine tuning and MOT coils the axial magnetic field has been measured as a function of \( z \). The measurements were taken at \( (x, y) = (0, 0) \) and \( I = 10 \pm 0.1 \) A. The Bias coils consist of 17 turns each. For the gradient coils the radial magnetic field gradient \( B' \) is given. The measurements are compared to the calculated values. Also the measured displacement of the minimum of the magnetic field \( d_0 \) is given in mm.

<table>
<thead>
<tr>
<th>Coil</th>
<th>Measurements</th>
<th>Calculations(^a)</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>( B_0 ) ( (G/A) )</td>
<td>( B' ) ( (G/Amm) )</td>
</tr>
<tr>
<td>Bias</td>
<td>-1.16</td>
<td>-0.00024</td>
</tr>
<tr>
<td>Pinch</td>
<td>1.01</td>
<td>-</td>
</tr>
<tr>
<td>Bias+Pinch(^c)</td>
<td>-0.133</td>
<td>-</td>
</tr>
<tr>
<td>Fine tuning</td>
<td>0.67</td>
<td>-</td>
</tr>
<tr>
<td>Gradient:</td>
<td></td>
<td></td>
</tr>
<tr>
<td>( B_z(y) )(^d)</td>
<td>-</td>
<td>0.035</td>
</tr>
<tr>
<td>( B_y(x) )(^d)</td>
<td>-</td>
<td>0.035</td>
</tr>
<tr>
<td>MOT</td>
<td>-</td>
<td>0.033</td>
</tr>
</tbody>
</table>

\(^a\)\(\S\) 2.4

\(^b\)Uncertainty is \( \pm 1.5 \) (mm).

\(^c\)Measured with Bias and Pinch coils connected in series.

\(^d\)Equation (2.13)
bias magnetic field of the Bias and the Pinch coils and the magnetic field curvature of the Bias and Fine tuning coils are about 10% lower than the calculated values. The bias magnetic field of the Fine tuning coils, the magnetic field curvature of the Bias and Pinch coils combined and the magnetic field gradient of the Gradient and MOT coils are about 15% lower than the calculated values. And the axial bias magnetic field of the Bias and Pinch coils combined and the magnetic field curvature of the Pinch coils are about 6% lower than the calculated values. These discrepancies are discussed in §2.7

2.5.4 Radial quadrupole magnetic field

Figure 2.11 shows the $y$-component of the Gradient magnetic field $B_y$ as a function of $x$ for different values of $y$ at $z = 4$ mm. In agreement with theory, $B_y$ increases linearly with $x$: $B_y = 0.035$ G/Amm. Similarly $B_x$ increases linearly with $y$. Both $B'_y$, $B'_x$, $x_0$ and $y_0$ are obtained from fitting the experimental data with either $B_x$ or $B_y$: 

$$B_x = B'_x \times (y - y_0),$$

$$B_y = B'_y \times (x - x_0),$$

(2.13)

where $\xi$ is either $x$ or $y$ and $\xi_0$ either $x_0$ or $y_0$.

Figure 2.12 shows the radial, $|B_r| = \sqrt{B_x^2 + B_y^2}$, and the $x-$ and $y-$components of the Gradient magnetic field as a function of $x$. From this figure it is clear that the $x-$component of the Gradient magnetic field $B_x$ is not entirely constant as a function of $x$ as it should be (A.6): $\frac{\partial B_x}{\partial x} = 0.005$ G/Amm. The fact that $\frac{\partial B_x}{\partial x} \neq 0$, could be explained by a slight and not unlikely tilt of the coil system with respect to the coordinate system of the magnetic field probe. This is depicted in Figure 2.13. When the coordinate system of the coils ($x'$- and $y'$-axis (dashed lines) in Figure 2.13) is rotated around the $z-$axis over an angle $\phi$ relative to the coordinate system of the probe ($x-$ and $y-$ axis (solid lines) in Figure 2.13), the measurements of $B_y$ as a function of $x$ could have been taken
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Figure 2.12: The x- and y- component and the radial Gradient magnetic field as a function of x at \((y, z) = (-8, -5)\) mm and \(I_y = 10\) A. The curves are fitted with either \(B_x = B'_x \times (y - y_0)\), \(B_y = B'_y \times (x - x_0)\) (2.13) or \(|B_r| = B'_r \times (r - r_0)\).

slightly off-axis by an angle \(\phi\). As a result the y-component of the magnetic field generated by the Gradient coils \(B_{G,y'}\), can be resolved in a \(B_x\) and \(B_y\) component of the magnetic field in the coordinate system of the probe, which we measure. Moreover, when moving the probe along the x-axis, in the coordinate system of the probe we not only move along the \(x'\)-axis but also along the \(y'\)-axis in the coordinate system of the coils. This results in a \(x\)-component of the magnetic field as function of \(x\) in the coordinate system of the probe \(B_x = B_{G,y'} \sin \phi = \frac{\partial B_x}{\partial x} x\). The measurements in Figure 2.12 are consistent with \(\phi = 8^\circ\).

The radial Gradient magnetic field \(|B_r|\), is depicted in Figure 2.14a as a function of \(r\). The relation between the absolute radial Gradient magnetic field and the radius \(r\) should be linear. However, a small turn near \(r = 8\) mm exists. Figure 2.14b shows the absolute radial Gradient magnetic field as a function of \(r + \Delta r\). Now \(|B_r|\) is indeed linearly dependent on \(r\). Apparently this irregularity is due to the uncertainty in determining the \(x\)-coordinate. Since \(y\) is kept constant for these measurements, \(\Delta r\) is only dependent on \(\Delta x\): \(\Delta r/\Delta x = x/r\).

When the origins of the coordinate systems of the probe and the coils do not coincide, the \(x\)-coordinate (in the coordinate system of the probe) is shifted relative to its true value, \(x'\) (in the coordinate system of the coils). This is a possibility, since the uncertainty in determining the center of the coil configuration is 1.5 mm. Besides we have seen that \(B_y = 0\) at \(x_0 = (2.5 \pm 1.5)\) mm, instead of \(x_0 = 0\) mm. When using the 'wrong' value of the \(x\)-coordinate, the wrong values of \(B_x\) and \(B_y\) are added, resulting in an incorrect value for \(|B_r|\). Correcting \(x\) with \(\Delta x = -1\) mm, yields the correct behaviour of \(|B_r|\) as a function of \(r\) (Figure 2.14b). The shift in \(x'\) due to the rotation of the coordinate system of the coils around the \(z\)-axis relative to the coordinate system of the probe

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Figure 2.13: Schematic picture of the consequences of a slightly off-axis scan along the $x$–axis. The $x$– and $y$–axis (solid lines) form the coordinate system of the probe. The $x'$– and $y'$–axis (dashed lines) form the coordinate system of the Gradient coils. Because of a slight tilt of the Gradient coils relative to the coordinate axes of the probe, the $y'$–component of the magnetic field generated by the Gradient coils $B_{G,y'}$ can be resolved in a $B_x$ and $B_y$ component of the magnetic field in the coordinate system of the probe.

Figure 2.14: Absolute radial Gradient magnetic field $|B_r|$, as a function of $r$ and $b\ r + \Delta r$ at $(y, z) = (-8, -5)\ mm$ and $I_g = 10\ A$. Here $r + \Delta r$ is the radius after correction of $x$ with $\Delta x = -1\ mm$. 

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Figure 2.15: Axial MOT magnetic field \( B_z \) as a function of \( z \) at \((x, y) = (0, 0)\) mm and \( I_m = 10 \) A. The measurement data are fitted with (2.11). The measurement was taken in the final coil configuration.

over an angle \( \phi = 8^\circ \), \( \Delta z = x(1 - \cos \phi) \), is negligibly small.

As shown in Table 2.5, \( B'_y = B'_x = 0.035 \pm 0.001 \) G/Amm. This is about 14% lower than the calculated value, which equals \( B' = 0.041 \) G/Amm. Furthermore, \( B_y \) is zero at \( z_0 = (2.5 \pm 1.5) \) mm, while measurements show (not shown here) that \( B_z \) is zero for \( y_0 = (0.3 \pm 1.5) \) mm. So, along the \( y \)--axis the zero point of the Gradient magnetic field coincides with the geometrical center of the trap, while along the \( x \)--axis this is not the case.

However, adjustments of a few millimeter in the position of the trap or the metastable neon beam are feasible (§ 3.4).

2.5.5 MOT magnetic field

Figure 2.15 shows the axial magnetic field of the MOT coils as a function of the \( z \)--coordinate at \((x, y) = (0, 0)\) mm and \( I_m = 10 \) A, where \( I_m \) is the current through the MOT coils. The gradient of the spherical magnetic quadrupole field equals \( B'_z = 0.033 \) G/Amm and \( B_z \) is zero at \( z_0 = -0.6 \) mm. From Table 2.5 we see that again the measured values are lower (by 13 %) than the calculated values.

The \( x \)-- and \( y \)--component of the MOT magnetic field decrease, respectively, linearly with the \( x \)-- and \( y \)--coordinate. The absolute value of the gradient of the magnetic field \( B'_{zi} \), \( i = x, y \), is in both cases equal to \( B'_z/2 \) (A.9). Here \( x_i \) is either \( x \) or \( y \). Measurements show that both \( B_z \) and \( B_y \) are constant as a function of \( z \). In addition \( B_z \) is constant as a function of \( x \) and \( y \). This is in agreement with theory (Appendix A.7).
2.6 Final coil configuration

In this section a summary is given of the measurements of the magnetic fields in the final coil configuration. With final coil configuration is meant the configuration of the coil in the final configuration. After these measurements the wooden dummy chamber only needs to be replaced by the vacuum chamber. This can only change the distance along the z-axis between two identical coils, the relative orientation between the different coils is not changed. In between these and the former measurements, described in the previous section, the coil configuration has been taken apart in order to attach temperature sensors to the coils. Also, the coils have been connected to the watercooling system. The current through the Clover Leaf coils is of the order of $200 - 300$ A, therefore the coils will heat up and need to be protected against overheating (the temperature characteristic of a Gradient coil is given in Appendix B). Moreover, two turns have been removed from each of the Bias coils, resulting in two Bias coils with 15 turns each. Since the relative position of the coils with respect to each other has a large effect on the generated magnetic fields, the magnetic fields of all the coils are measured again in the final coil configuration.

The results are given in Table 2.6. The measurements were done in the same geometry of the experimental setup and with the same Hall probes as in the previous measurements (§ 2.5.1). But now, a one-dimensional Stepper Motor is used and the output voltage of the Hall probe is converted by a 12-bit single mode DAS and read by a PhyDas interface. The magnetic field has been measured.
Table 2.6: Measured values of the magnetic field, per Ampère for each coil in the final coil configuration. For the Bias, Pinch, Fine tuning and MOT coils the axial magnetic field has been measured as a function of \( z \). The measurements were taken at \((x, y) = (0, 0)\) and \( I = 75 \pm 0.1\) A For the gradient coils the radial magnetic field gradient \( B' \) is given. Also the measured displacement \( d_0 \) of the minimum of the magnetic field is given in mm. For the Gradient coils \( d_0 \) is either equal to \( x_0 \) or \( y_0 \). In all other cases \( d_0 = z_0 \). Between these and the former measurements two turns have been removed from the Bias coils. The Bias coils now consist of 15 turns each.

<table>
<thead>
<tr>
<th>Coil</th>
<th>( B_0 ) (G/A)</th>
<th>( B' ) (G/Amm)</th>
<th>( B'' ) (G/Amm(^2))</th>
<th>( d_0 \pm 1.5 ) (mm)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Bias(^a)</td>
<td>-0.977</td>
<td>-</td>
<td>-0.000254</td>
<td>0.1</td>
</tr>
<tr>
<td>Pinch</td>
<td>0.920</td>
<td>-</td>
<td>0.0047</td>
<td>-0.7</td>
</tr>
<tr>
<td>Bias+Pinch(^b)</td>
<td>0.0084</td>
<td>-</td>
<td>0.00474</td>
<td>0.25</td>
</tr>
<tr>
<td>Fine tuning</td>
<td>0.716</td>
<td>-</td>
<td>0.0016</td>
<td>1.4</td>
</tr>
<tr>
<td>MOT</td>
<td>-</td>
<td>0.033</td>
<td>-</td>
<td>-1.2</td>
</tr>
<tr>
<td>Gradient</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>( B_x (y) )</td>
<td>-</td>
<td>0.0331</td>
<td>-</td>
<td>0.04</td>
</tr>
<tr>
<td>( B_y (x) )</td>
<td>-</td>
<td>0.0335</td>
<td>-</td>
<td>-1.13</td>
</tr>
</tbody>
</table>

\(^a\)Consisting of 15 turns.
\(^b\)Measured at \( I = 200\) A, while the Bias and Pinch coils were connected in series.

along all axes with a resolution of \( 0.62 \pm 0.02\) mm. The measurements are operated/controlled by a Labwindows program.

The signal of the probe has not been amplified, since the measurements were done at much larger currents (75 or 100 A) and thus much larger magnetic fields. This was previously not possible because the watercooling of the coils had not been implemented yet. The uncertainty in the measured values is equal to 6%, due to the sensitivity of the probe of 2% and the uncertainty of 4% in the stepsize of the Stepper Motor.

Comparing Table 2.5 and 2.6, we observe that the values of the bias magnetic field \( B_0 \) for the Bias \((N = 15)\) and Pinch coils are, respectively, 12 % and 20 % lower than the calculated values. Also the radial magnetic field gradient of the Gradient coils, \( B' \), is about 20 % lower than the calculated value.

On the other hand, the axial bias magnetic field and the magnetic field curvature \( B'' \) of the Fine tuning coils are higher than the previously measured values and the magnetic field gradient \( B' \) of the MOT coils is the same for both measurements. In short the measured values in the final coil configuration are, within the 6 % uncertainty of the measurements, about 15 % lower than the calculated values, just like the previous measurements. So the former measurements and these measurements in the final coil configuration are consistent with each other.

Due to the uncertainty of 6 % in the magnetic field measurements, it is impossible to derive the combined axial bias magnetic field of the Bias and Pinch coils from the separate measurements for each coil. According to Table 2.6 the total axial bias magnetic field of the Bias and Pinch coils combined is \(-11.4\) G. Due to the uncertainty of 6 %, however, their combined magnetic field could lie anywhere between \(-34.2\) and \(11.4\) G. Therefore the Bias and Pinch coils are connected in series and
Figure 2.16 shows the total axial magnetic field of the Bias and Pinch coils combined. The coils are connected in series and the current through the coils is equal to \( I = 200 \) A. The total bias magnetic field, \( B_{t,0} = +1.68 \) G, is positive and of the order of 1 G (2.7), meeting the trapping requirements (§ 1.4.2). As expected, the curvature of the magnetic field is entirely determined by the curvature of the Pinch coils.

While transferring the atoms from the MOT to the MT, the total bias magnetic field of the Bias and Pinch coils should be of the order \( \sim 100 \) G (Table 2.2), thereby creating a weaker trap with a smaller trap depth. Therefore, the current through the Bias coils (and thus the Bias magnetic field) is reduced to \( I_b = 117 \) A during the loading phase. For \( I_b = 117 \) A and \( I_p = 200 \) A, the total axial bias magnetic field is equal to:

\[
B_z(z)[G] = 70[G] + 0.94[G/mm^2] \times z^2[mm^2],
\]

using the values of Table 2.6.

2.7 Discussion and conclusions

From the results presented above it can be concluded that the magnetic fields in the final coil configuration meet the trapping requirements. In addition, it is clear that the measured magnetic field values are systematically 2 - 15 % lower than the corresponding calculated values for all coils. This is not due to a badly calibrated probe. Taking all the uncertainties in the calculations and the measurements into account, they might account for the discrepancy of 2 - 15 % between the measurements and the calculations. The source of these uncertainties are discussed in the next paragraphs.

First, the uncertainty in the magnetic field measurements is equal to 2 % (sensitivity Hall probe) for the measurements presented in § 2.5 and 6 % for the measurements in the final coil configuration. Second, it was shown that the uncertainty of 1 mm in the coil parameters \( A \) and \( R \) results in an uncertainty of, respectively, 2 % and 16 % in the calculated axial bias magnetic field \( B_0 \) for the Bias and the Pinch coils at \( I = 200 \) A, and an uncertainty of, respectively, 25 % and 33 % in the calculated axial magnetic field curvature \( B'' \). The corresponding uncertainty in the calculated MOT magnetic field gradient is 6 % at \( I_M = 30 \) A.

Third, a possible error in the thickness of the coils of 0.5 mm might lead to an uncertainty of 1 - 2 % in the magnetic field parameters. Fourth, approximating each turn by a circular loop of wire in the calculations of the magnetic fields, might introduce an uncertainty of 2 %.

Moreover, in calculating the radial magnetic field gradient of the Gradient coils, the complex structure of the coils is approximated by two elliptical and two straight line segments for each coil (Figure A.2). An uncertainty of 15 % is then maybe not so surprising.

In addition, it is difficult to determine the exact location of the geometrical center of the Clover Leaf coil configuration. The uncertainty in determining the location of the geometrical center is estimated to be \( \approx 1.5 \) mm. Therefore it is difficult to see if the points where respectively the magnetic field of the Gradient and MOT coils are zero do overlap and if these points coincide with the geometrical center of the trap. It is important that this is the case within a certain margin, because the atoms cannot be trapped when they do not pass through the center of the MOT and Clover Leaf trap.

Fortunately adjustments of the order of \( \pm 5 \) mm can be made in the relative position of the zero of the magnetic field of the MOT and MT. Furthermore the bright, cold metastable Neon beam can
be adjusted over a few mm inside the trap. And because the diameter of the MOT beams is 20 mm, a small (~1 mm) displacement of the zero of the magnetic field of the MOT clearly does not pose a problem.
Chapter 3

Magneto-Optical Trap

3.1 Introduction

To obtain a BEC not only a very bright cold atomic beam is required, but the atoms also have to be captured and cooled to temperatures below the critical BEC temperature in a trap. Therefore, we load our bright cold atomic beam successively into a Magneto-Optical trap (MOT) and a Magneto-static trap (MT).

Our Ne* MOT is the first accomplished at Eindhoven University of Technology and the largest accomplished ever. Only Shimizu et al [30] have realized a Ne* MOT so far. His Ne* MOT, however, only contained $4 \times 10^7$ atoms at the maximum.

In the MOT the trapped atoms can only be cooled to the sub-Doppler temperature limit, which lies in the $10 \mu$K regime. Therefore, the atoms will be successively transferred to the MT to cool them to temperatures below the critical BEC temperature. The cooling process in the MT works most efficiently, however, when the atoms are first cooled to as low as possible temperatures in the MOT. In order to understand the capture and cooling processes in the MOT, first the laser cooling processes in the MOT are briefly explained in § 3.2.

In § 3.3 the loading phase of the MOT and characteristic loss processes in the MOT are discussed. Third, in § 3.4 the experimental setup is briefly discussed. Next in § 3.5 two measurement techniques for measuring the number of particles, the particle density etc. are explained. Then in § 3.6, first measurements on the number of particles, the particle density and the loss rate due to ionization in the MOT, are presented. Finally, some conclusions are given in § 3.7.

3.2 Laser cooling

3.2.1 Introduction

In the MOT different cooling processes play a role. Immediately after loading the relatively 'hot' atoms into the MOT, Doppler cooling forces are most important. The principle of Doppler cooling is described in subsection 3.2.2. The trapping principle of the MOT based on these Doppler forces is briefly described in subsection 3.2.3. The temperature to which atoms can be cooled, using Doppler cooling, is limited. However, when the atoms are cooled to temperatures around the Doppler limit,
they can be cooled to even lower temperatures using polarization gradient forces. The principle of these so-called sub-Doppler forces is briefly explained in subsection 3.2.4.

The absolute temperature limit to which atoms can be cooled using light fields is the recoil limit, which is given in subsection 3.2.5. To conclude this section, the limiting density in the MOT, due to the balance between attractive and repulsive forces in the MOT, is briefly discussed in subsection 3.2.6.

3.2.2 Doppler cooling

Laser cooling is based on the recoil kick of the photons in a laser beam. Imagine an atom with velocity $\vec{v}_0$ moving in a slightly red-detuned, $\delta = \omega_L - \omega_0 < 0$, counter-propagating, running light wave. Here $\delta$ is the detuning of the laser, $\omega_0$ the resonance frequency of the atomic transition and $\omega_L$ the laser frequency. Due to the Doppler effect, the frequency of the counter propagating light wave $\omega_L = \omega_0 + \delta$ is Doppler shifted to higher frequencies from the atoms point of view: $\omega = \omega_L + \Delta \omega_D$. Here $\Delta \omega_D = \vec{k} \cdot \vec{v}_0$ is the Doppler shift. Whenever the (negative) detuning of the laser matches the (positive) Doppler shift $\delta = \Delta \omega_D$, the atom is resonant with the laser light and absorbs a photon.

Since momentum is conserved, the absorption or emission of a photon changes the atomic velocity by one recoil velocity $v_{\text{recoil}} = \hbar k / m = 3.1$ cm$^{-1}$, where $k = 2\pi / \lambda$ is the wave number of the laser beam and $m$ the atomic mass. For each photon absorbed the atomic velocity is changed by one recoil velocity $V_{\text{recoil}} = \frac{\hbar k}{m} = 3.1$ cm$^{-1}$, where $k = 2\pi / \lambda$ is the wave number of the laser beam and $m$ the atomic mass. For each photon absorbed the atomic velocity is changed with $-V_{\text{recoil}}$ in the direction of the laser propagation. The absorbed photons are subsequently randomly emitted by the atom, so no net change in the atomic velocity occurs due to these spontaneously emitted photons. As a consequence, the scattering force on the atom is equal to the photon scattering rate times the photon momentum. For a two-level atom in a running wave this force is given by [15]:

$$\vec{F} = -\hbar k \frac{\Gamma}{2} \frac{s_0}{1 + s_0 + (2(\omega - \omega_0) / \Gamma)^2},$$

where $\Gamma$ is the natural line width of the transition and $s_0$ is the saturation parameter at resonance, defined as [15]:

$$s_0 = \frac{I}{I_0},$$

with $I$ the intensity of the laser beam and $I_0$ the saturation intensity. The saturation parameter of the transition is defined as:

$$s = \frac{s_0}{1 + (2\delta / \Gamma)^2},$$

with $\delta = \omega - \omega_0$ the detuning of the light perceived by the atom from resonance.

Summarizing, the Doppler shift and the detuning of the laser combined, create a velocity dependent force. The maximum scattering force which can be exerted on an atom in this way equals [15]:

$$F_{\text{max}} = -\frac{\hbar k \Gamma}{2}.$$

For the Ne$^*$ $|^3P_2, m_J = 2\rangle \leftrightarrow$ Ne$^{**}$ $|^3D_3, m_J = 3\rangle$ transition this maximum force is equal to: $F_{\text{max}} = -2.665 \times 10^{-20}$ N, corresponding to an acceleration of $a = -8.027 \times 10^5$ ms$^{-2}$.
When the atom is moving in an inhomogeneous magnetic field, the frequency which the atom perceives, will obtain an extra shift due to the Zeeman effect (1.4):

\[ \Delta \omega_z = \Delta E_e - \Delta E_g = \frac{\mu_B B_{\text{ext}} (m_J g_J e - m_J g_J g)}{\hbar}, \]  

(3.5)

when \( B_{\text{ext}} \) is aligned along the quantization axis. For the Ne\(^+\) \( ^3P_2, m_J = 2 \) \( \leftrightarrow \) Ne\(^++\) \( ^3D_3, m_J = 3 \) transition, \( m_J g = 2, m_J e = 3, g_J g = 3/2 \) and \( g_J e = 4/3 \), yielding: \( \Delta \omega_z = \frac{\mu_B B_{\text{ext}}}{\hbar} \), or 1.4 MHz/G.

In this way a position dependent force can be exerted on the atoms by a position dependent magnetic field, like a quadrupole field. Thus the force on an atom depends on the total shift of the frequency which the atom perceives with respect to the resonance frequency of the transition \( \Delta \omega = \omega - \omega_0 = \delta + \Delta \omega_D + \Delta \omega_z \). The atom is resonant with the laser light, when the total frequency shift \( \Delta \omega \) is zero.

Due to the natural line width \( \Gamma \) of the atomic excited state, this process will take place for each atom moving with a velocity within the velocity capture range \( \Delta v \) around \( v_0 \):

\[ k \Delta v \sim \Gamma \]  

(3.6)

If the velocity of the atom lies outside this velocity capture range the absorption rate of photons will be much smaller. For the Ne\(^+\) \( ^3P_2, m_J = 2 \) \( \leftrightarrow \) Ne\(^++\) \( ^3D_3, m_J = 3 \) transition this velocity capture range is equal to \( \Delta v \sim 5.25 \) m/s.

It is crucial for this process to work efficiently that the atom is effectively a so-called two level atom, so that the atom relaxes always to the same atomic state and the above described absorption and emission cycle can be repeated many times. The Ne\(^+\) \( ^3P_2, m_J = 2 \) and Ne\(^++\) \( ^3D_3, m_J = 3 \) excited states form such a two level system (§ 1.3).

The method described above can be used to slow atoms moving in one direction. Atoms moving in the opposite direction, however, are not slowed. This problem can be solved by using two counter propagating laser beams, also known as one-dimensional optical molasses. In the low intensity limit \( s \ll 1 \), for a negative detuning \( \delta < 0 \) and \( |\Delta \omega_D| \ll (\Gamma, \delta) \), the effective force on the atom is the sum of the forces of the two counter propagating laser beams and is equal to a friction constant \( \beta \) times the velocity of the atoms. This friction constant \( \beta \) is defined as [15]:

\[ \beta = -\hbar k^2 \frac{8s_0 (\delta/\Gamma)}{(1 + (2\delta/\Gamma^2))^2}. \]  

(3.7)

So this force is a continuous damping force, proportional to the velocity of the atom, which cools the atom towards zero velocity.

But because diffusional heating competes with the damping of the velocity, due to the above described process of Doppler cooling, the temperature to which the atoms can be cooled is limited. This limit is called the Doppler limit. The diffusional force is due to fluctuations in the number and direction of the emitted photons and causes a broadening of the velocity distribution or diffusional heating. This diffusional force can be characterized by a diffusion constant \( D \). Both forces together describe a 'random walk' process which is characterized by a steady-state equilibrium temperature [15]:

\[ k_B T = \frac{D}{\beta} = \hbar \left( \frac{\Gamma^2/4 + \delta^2}{-2\delta} \right). \]  

(3.8)
This equilibrium temperature (3.8) is minimum for \( \delta = -\Gamma /2 \), yielding the so-called Doppler limit to which the atoms can be cooled:

\[
k_B T_D = \hbar \Gamma /2.
\]

(3.9)

For the Ne* \( |^3P_2, m_J = 2 \rangle \leftrightarrow |^3D_3, m_J = 3 \rangle \) transition the Doppler limit is equal to \( T_D = 196 \mu \text{K} \), corresponding to a rms velocity of \( v_D = 0.29 \text{ ms}^{-1} \).

Because of the coupling between the laser field and the atom, the energy levels of the 'ground' and excited state of the atom are shifted by a light shift \( \Delta \). As a result the 'ground' and excited state are mixed in so-called dressed states. It can be shown that the light shifted energies of the 'ground' \( E_g \) and the excited state \( E_e \), are given by [15]:

\[
E_g = \hbar \Delta_g = +\frac{\hbar \delta}{2} \times C^2,
\]

\[
E_e = \hbar \Delta_e = -\hbar \delta (1 + \frac{\delta}{2}) \times C^2,
\]

(3.10)

where \( C \) is the Clebsch-Gordon Coefficient (C.4). For the Ne* \( |^3P_2, m_J = 2 \rangle \leftrightarrow |^3D_3, m_J = 3 \rangle \) transition with a detuning of \( \delta = -5\Gamma \) and a saturation parameter of \( s_0 = 0.5(2) \), this relation yields: \( \Delta_g = -10.1(-40.6) \times (2\pi) \times 10^4 \text{ Hz} \) and \( \Delta_e = +41.1(41.4) \times (2\pi) \times \text{MHz} \).

3.2.3 Trapping principle of the MOT

The trapping force of the MOT is explained in Figure 3.1a and b for a simplified one-dimensional case with \( J = 0 \). The quadrupole field of the MOT in combination with two counter propagating laser beams, constitutes the trapping force. A right hand circularly polarized \( \sigma^+ \) running light wave moves from the left to the right. A left hand circularly polarized \( \sigma^- \) running light wave comes from the right. The quadrupole field of the MOT is zero in the origin of the setup and increases linearly outwards. This inhomogeneous magnetic field induces a spatially dependent Zeeman shift (1.4) in the atomic levels (\( m_L = 1 \) and \( m_L = -1 \)). As a result an atom at the left of the origin will be more resonant with \( \sigma^+ \) light coming from the left, and will experience a force that pushes it towards the origin. Similarly, an atom at the right side of the origin will be pushed back towards the origin by the \( \sigma^- \) light, travelling from the right to the left. Figure 3.1b) shows the resulting position dependent trapping force as a function of \( z \). Three of these pairs of counterpropagating laser beams constitute a three-dimensional trapping force.

3.2.4 Sub-Doppler cooling

Introduction

The temperature of the atom cloud in a three dimensional molasses can be reduced to values lower than the Doppler limit (3.9) by using polarization gradient forces. These radiative forces are based on nonadiabatic couplings between Zeeman levels undergoing different light shifts. As a consequence these radiative forces only give a significant contribution when the light shift (3.10) is greater than the Zeeman shift (3.5) of the atomic levels. Therefore sub-Doppler cooling only occurs when the Zeeman shift and Larmor precession do not exceed the light shift or interfere with the optical pumping among the magnetic sublevels. In the MOT the spherical quadrupole field and, thus the Zeeman shift, is zero.
Figure 3.1: Trapping principle of the MOT, a the Zeeman shift and b the resulting trapping force as a function of the $z$-coordinate. The Zeeman effect, due to the quadrupole magnetic field, causes a shift in the atomic levels. As a result the resonance frequency of a transition between two states (here $L = 0$ and $L = 1$) changes as a function of space. An extra Zeeman detuning is the result. This change in detuning as a function of space brings the atoms into resonance with the red-detuned laser light, at certain positions in space. The resultant force, (Figure b), can be modeled with a box potential, if the gradient of the magnetic field and the detuning of the laser light are relatively large.
at the center of the trap. Therefore these so-called polarization gradient forces play an important role at the center of the trap where the atom cloud is confined.

In a one-dimensional standing wave three processes give rise to a radiation force associated with a gradient of polarization. First, in the $\sigma^+ - \sigma^-$ configuration (two opposed counter propagating beams of either $\sigma^+$ or $\sigma^-$ polarization, like in the MOT, Figure 1.2) the induced orientation effect plays an important role. Second, in the $\perp \perp$ configuration (two counter propagating beams with mutually perpendicular linear polarizations), the Sisyphus effect occurs. Third, in stronger magnetic fields also velocity sensitive magnetic resonances (VSR) occur in both configurations. In general, a mixture of these polarization gradient forces exists in the MOT. The trap can, however, be divided into two regions: the central low-field region, where only the induced orientation effect is significant, and the surrounding high-field region, where the velocity selective resonance (VSR) is dominant. Since the trapped atoms are confined in the low-field region, the high-field region is only important for the capture process. Here, we will only briefly discuss the induced orientation effect.

**Induced Orientation effect**

Two internal times are important for atoms that have various Zeeman sublevels $|J,m_J\rangle$, such as neon. The radiative lifetime $\tau_r = \frac{1}{\Gamma}$, where $\Gamma$ is the natural width of the excited state, and the optical pumping time $\tau_p = \frac{1}{S}$, characterizing the mean time that it takes for an atom to be transferred by a fluorescence cycle from one sublevel $|J,m_J\rangle$ to another $|J',m_J\rangle$. Here $S$ is the mean scattering rate of incident photons and is for a steady state defined as [15]:

$$S = \frac{\Gamma}{2}. \quad (3.11)$$

The optical pumping between the different Zeeman sublevels is the origin of the sub-Doppler forces.

In the limit of high intensities of the laser radiation field, absorption and emission cycles on a timescale $\tau \ll 1/\Gamma$, result in an oscillating occupation of the ground and excited state levels. Or in other words, the transition probability oscillates as a function of time. The frequency of this oscillation is the so-called Rabi-frequency $\Omega$, which is defined as [15]:

$$\Omega = \langle \epsilon | d_{LM} | g \rangle \frac{E_0}{\hbar}, \quad (3.12)$$

where $E_0 = \sqrt{I/(\epsilon_0 c)}$ is the amplitude of the electric field with $I$ the intensity of the laser. For a standing wave of circularly polarized light the amplitude of the electric field is equal to $\sqrt{2}E_0$. For the Ne* $|3P_2,m_J = 2\rangle \leftrightarrow |3D_3,m_J = 3\rangle$ transition induced by $\sigma^+$ photons, the Rabi-frequency at resonance and $I = I_0 = 4.08 \text{ mWcm}^{-2}$ is equal to $5.79(2\pi) \text{ MHz} = \frac{\Gamma}{\sqrt{2}}$.

At low laser power, when the Rabi frequency $\Omega$ (3.12) is small compared to $\Gamma$, $\tau_p \gg \tau_r$ and thus $\Gamma' \ll \Gamma$. In this case, nonadiabatic effects occur at much smaller velocities $kv \sim S$ than those required for Doppler cooling ($kv \sim \Gamma$ (3.6)). So large friction forces can only be experienced by very slow atoms.

In addition, long pumping times $\tau_p$ can only give rise to large friction forces, if the occupation of the atomic states strongly depends on the position of the atom in the laser beam [7]. This position dependent difference in the occupation of the atomic levels results from the existence of large population differences among the Zeeman sublevels $|J,m_J\rangle$, or from coherences among these sublevels. Polarization gradients provide these spatial variations in the occupation of the atomic levels.
In the $\sigma^+ - \sigma^-$ configuration in one-dimensional molasses, the polarization vector rotates when one moves along the standing wave, but it keeps the same ellipticity. The laser polarization is always linear and the laser intensity is the same for all $z$ (Appendix D Figure D.1). Therefore, the light shifted energies, which are proportional to the light intensity, do not vary as a function of $z$.

But the transition probabilities between different Zeeman sublevels differ and atoms will concentrate in a certain sublevel (Appendix C, Figure C.1). Because the light shift is directly proportional to the intensity of the transition, the Zeeman sublevels will have different light shifts. As a result, the wave functions vary as a function of $z$ and nonadiabatic couplings could occur among the various Zeeman sublevels undergoing different light shifts.

A cumbersome analysis [7] shows that for moving atoms, the populations of the $|J, \pm m_J\rangle$ states are no longer identical. This motion-induced population difference between the sublevels causes an imbalance in the radiation pressure and the velocity of the atoms will be damped.

The temperature to which the trapped Ne* atoms in the MOT can be cooled with polarization gradient forces for $s_0 = 0.5$ and $\delta = -5\Gamma$ is:

$$T_{\text{sub}} = 4.3 \, \mu\text{K}. \quad (3.13)$$

A brief summary of the derivation of this sub-Doppler limit is given in Appendix D. The experimentally observed limit is usually of the order of $\sim 40 \, \mu\text{K}$. The time necessary to cool the atoms to this temperature is equal to:

$$\tau = 1.5 \, \text{ms}. \quad (3.14)$$

### 3.2.5 Recoil limit

The absolute temperature limit to which atoms can be cooled with light fields is the recoil limit, due to the absorption of at least one photon. The recoil limit is defined as:

$$k_BT_R = \frac{\hbar^2 k^2}{2m}. \quad (3.15)$$

For the Ne* $|^3P_2, m_J = 2\rangle \leftrightarrow |^3D_3, m_J = 3\rangle$ transition, the recoil limit is equal to $T_R = 1.17 \, \mu\text{K}$, corresponding to a rms velocity $v_R = 2.2 \, \text{cm/s}$.

### 3.2.6 Scattering force and limiting density

Due to their thermal motion, trapped atoms spread out to a root mean square (rms) radius $r$ given by the equipartition theorem:

$$\frac{1}{2}k_BT = \frac{1}{2}\kappa(r^2). \quad (3.16)$$

When more atoms are loaded into the trap at a given equilibrium temperature $T$ the rms radius of the cloud remains constant, while the density increases. This increase in density is limited by repulsive forces between the atoms. The density is then determined by the relative magnitude of the repulsive forces and the spring constant $\kappa$ of the trap.

These repulsive forces result from the scattering of photons from one atom (1) to another (2) in the trap and the subsequent absorption of these scattered photons by the latter (2) atom. Also an attractive force is present between the atoms in the trap, because atoms at the edge of the atom cloud...
will attenuate the incoming MOT laser beams and thus produce an intensity imbalance that tends to compress the cloud.

The limiting density distribution of the trapped atom cloud is now determined by the balance between the attractive force, the repulsive scattering force and the trapping force \(-\kappa r\). Spherical symmetry and a two-level atom are assumed for simplicity. It can be shown that the uniform limiting density distribution \(n_{\text{limit}}\) is given by [1]:

\[
\frac{3\kappa c}{1 + \sigma_a} 
\]

Here \(\kappa = \kappa_{\text{ind}}\) the spring tensor of the induced orientation effect (D.5), which is the dominant cooling process at the center of the trap, \(\sigma_R\) the cross section for an atom (2) to absorb the reradiated photons of another atom (1), and \(\sigma_a\) the cross section for absorption of photons from the laser field. The only unknown parameter in this formula is \(\sigma_R/\sigma_a\). The cross section for absorption of the laser light is given by [15]:

\[
\sigma_a (\omega - \omega_0 ) = (J g m_a L M | J_e m_e )^2 \frac{\lambda^2}{2\pi} \frac{1}{\Gamma^2} \left( \frac{\omega - \omega_0}{\Gamma} \right)^2.
\]

Here \(\Gamma_{eg}\) is the spontaneous decay rate from excited to ground state, which is equal to the total spontaneous decay rate \(\Gamma\) in a two-level system. The parameter \(\lambda\) is the wavelength of the atomic transition and the transition probability for the Ne* \(|^3P_2, m_J = 2\) \(\leftrightarrow \text{Ne}^{**} |^3D_3, m_J = 3\) transition is equal to \((J g m_a L M | J_e m_e )^2 = 1\) (Appendix C).

The cross section for absorption of reradiated light \(\sigma_R\) consists of two contributions: an elastic contribution equal to \(\sigma_a\) and an inelastic (fluorescence) contribution. The cross section for absorption of the inelastically scattered light can be approximated by the cross section for absorption of the laser light \(\sigma_a\) at zero detuning [1]. Because the ratio of the intensity of the elastically scattered light and the total scattered light intensity is \(\frac{1}{s+1}\), we obtain [1]:

\[
\frac{\sigma_R}{\sigma_a} - 1 \approx \left( \frac{s}{s+1} \right) \frac{\delta^2}{s(\delta^2 + \Gamma^2/4) + \Gamma^2/4}.
\]

For the Ne* \(|^3P_2, m_J = 2\) \(\leftrightarrow \text{Ne}^{**} |^3D_3, m_J = 3\) transition, and a laser beam with detuning \(\delta = -5\Gamma\) and a saturation parameter of \(s_0 = 0.5\) (\(s_0 = 2\)), \(\frac{\sigma_R}{\sigma_a} - 1\) is equal to 0.33 (0.65). The limiting density (3.17) is then equal to:

\[
\frac{3\kappa c}{1 + \sigma_a} = 9.8 \times 10^{13} \text{cm}^{-3} (1.25 \times 10^{13} \text{cm}^{-3}).
\]

### 3.3 Loading the MOT

In order to load the slowed atoms into the MOT and to be able to successively cool them in the MT to temperatures below the critical BEC transition temperature, the lifetime of the MOT \(\tau\) must at least be longer than the time required to transfer the atoms from the MOT to the MT.
Table 3.1: Characteristic parameters of the radiation field and laser cooling for the \( \text{Ne}^* |^3 P_2, m_J = 2 \rangle \leftrightarrow \text{Ne}^* |^3 D_3, M_J = 3 \rangle \) transition.

<table>
<thead>
<tr>
<th>Quantity</th>
<th>Symbol</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Radiation field</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Saturation intensity</td>
<td>( I_0 )</td>
<td>4.08 mWcm(^{-2})</td>
</tr>
<tr>
<td>Rabi frequency(^a)</td>
<td>( \Omega )</td>
<td>5.79 (2(\pi)) MHz</td>
</tr>
<tr>
<td>Absorption cross section(^b)</td>
<td>( \sigma_a )</td>
<td>1.94 \times 10^{-15} m(^2)</td>
</tr>
<tr>
<td>Light shift (</td>
<td>^3 P_2 \rangle ) state (^6)</td>
<td>( \Delta _p )</td>
</tr>
<tr>
<td>Laser cooling</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Maximum Doppler acceleration</td>
<td>( a_{\text{max}} )</td>
<td>-8.1 \times 10^5 ms(^{-2})</td>
</tr>
<tr>
<td>Zeeman shift</td>
<td>( \Delta \omega_Z )</td>
<td>1.4 MHzG(^{-1})</td>
</tr>
<tr>
<td>Magnetic moment</td>
<td>( \mu = 3\mu_B )</td>
<td>2.78 \times 10^{-23} Am(^2)</td>
</tr>
<tr>
<td>Velocity capture range</td>
<td>( \Delta v )</td>
<td>5.25 ms(^{-1})</td>
</tr>
<tr>
<td>Doppler limit</td>
<td>( T_D )</td>
<td>196 (\mu)K</td>
</tr>
<tr>
<td>Doppler rms velocity</td>
<td>( v_D )</td>
<td>0.29 ms(^{-1})</td>
</tr>
<tr>
<td>Sub-Doppler limit</td>
<td>( T_{\text{sub}} )</td>
<td>4.35 (\mu)K</td>
</tr>
<tr>
<td>Sub-Doppler rms velocity</td>
<td>( v_{\text{sub}} )</td>
<td>4.3 cm(^{-1})</td>
</tr>
<tr>
<td>Recoil limit</td>
<td>( T_{\text{recoil}} )</td>
<td>1.2 (\mu)K</td>
</tr>
<tr>
<td>Recoil rms velocity</td>
<td>( v_R )</td>
<td>2.2 cm(^{-1})</td>
</tr>
<tr>
<td>Recoil velocity</td>
<td>( v_{\text{recoil}} )</td>
<td>3.1 cm(^{-1})</td>
</tr>
<tr>
<td>Cooling time(^c)</td>
<td>( \tau_{\text{ind}} )</td>
<td>1.5 ms</td>
</tr>
<tr>
<td>Limiting density(^b)</td>
<td>( \eta_{\text{limit}} )</td>
<td>5 \times 10^{11} cm(^{-3})</td>
</tr>
</tbody>
</table>

\(^a\delta = 0 \text{ and } s_0 = 1.\)

\(^b\delta = -5\delta \text{ and } s_0 = 0.5.\)

\(^c\delta = -5\delta \text{ and } s_0 = 0.5 \text{ and } \frac{\partial R}{\partial y} = 1 \text{ G/mm}.\)
The intensity of the Gemini beam line is \( I \approx 5 \times 10^{10} \) atoms s\(^{-1}\). The evolution of the number of particles in the trap as a function of time is given by [1]:

\[
\frac{dN}{dt} = I - \kappa_{\text{gas}} N n_{\text{gas}} - \kappa_{\text{ion}} \frac{N^2}{V} = I + \left( \frac{dN}{dt} \right)_{\text{gas}} + \left( \frac{dN}{dt} \right)_{\text{ion}},
\]

where \( \kappa_{\text{gas}} \) is the rate constant for collisions with the background gas, \( N \) the number of particles in the MOT, \( n_{\text{gas}} \) the density of the background gas, \( \kappa_{\text{ion}} \) the rate constant for ionization and \( V \) the trapping volume of the MOT.

For the alkali gases, collisions with the background gas (residual gases in the vacuum system) determine the lifetime of the MOT. A typical rate constant for collision with the background gas is [3]: \( \kappa_{\text{gas}} = 1.6 \times 10^{-9} \) cm\(^3\) s\(^{-1}\). At a characteristic background pressure of \( 10^{-9} \) Torr and a characteristic background gas temperature of 300 K, the trapping time, due to these collisions is \( \tau_{\text{gas}} = N/(dN/dt)_{\text{gas}} \approx 20\) s.

In trapped samples of rare gas atoms, like neon, on the other hand, ionization is an important loss process (§ 1.5). The loss rate of atoms from the trap, due to ionization, is directly proportional to the density squared (3.21). Therefore, it is important to have a sufficiently large MOT with a relative low density, to reduce trap losses due to ionization. For the unpolarized atoms in the MOT the ionization rate constant is estimated at (1.7): \( \kappa_{\text{ion}} \approx 5 \times 10^{-11} \) cm\(^{-3}\) s\(^{-1}\) [23]. But this is only a lower limit. When also light assisted Ne\(^*\) (3s) - Ne\(^*\)\(^{\text{2p}}\) collisions occur, the ionization rate constant is much larger.

If we take only loss due to ionization into account, and assume that we have at least \( 10^{10} \) atoms in our MOT after a loading time of \( t \approx 1\) s, the minimum trapping volume of the MOT should be [34]: \( V \geq 0.1 \) cm\(^3\). Since the axial MOT magnetic field gradient is twice as strong as the magnetic field gradient in the \( x-\) and \( y-\)direction, the dimension of the trap \( l \) in the \( z-\)direction is half as large as the dimension of the trap in the \( x-\) and \( y-\)direction \( l_x = l_y = 2l_z = 5.8\) mm. For this trapping volume the density equals \( 10^{11}\) cm\(^{-3}\) and the trapping lifetime due to ionization is \( \tau_{\text{ion}} = N/(dN/dt)_{\text{ion}} = 0.2\) s.

These values clearly show that the ionization decay time is much shorter than the trapping lifetime due to collisions of the trapped Ne\(^*\) atoms with the background gas. In addition, the trapping time due to ionization is also shorter than the lifetime of the metastable state, \( \tau = 24\) s. Thus ionization fully determines the lifetime of the metastable neon trap.

### 3.4 Experimental setup

The cold, bright atomic beam used for loading the MOT is supplied by the Gemini atomic beam machine of the group of Theoretical and Experimental Atomic Physics and Quantum Electronics of the Physics Department of the Eindhoven University of Technology. The Gemini beam machine consists of different cooling and beam brightening stages. Beam brightening, the increase in flux-rate of the metastable neon atoms, is necessary because the relative population of the metastable states in a gas discharge or an atomic beam is only a fraction of \( 10^{-4} \) of the total density (§ 1.4).

In subsection 3.4.1 the different cooling stages are briefly outlined and the characteristics of the generated bright, cold atomic beam are given. In subsection 3.4.2 the trapping chamber, consisting of the MOT and MT, and the beam diagnostics, are discussed.
Figure 3.2: Drawing of the Gemini atomic beam line. All five cooling stages and the trapping chamber are indicated.

3.4.1 Gemini atomic beam machine

A liquid nitrogen cooled, discharge-excited, supersonic expansion supplies metastable neon atoms in the $^3P_2$ state with an initial axial velocity of 500 m/s, a FWHM of 200 m/s and a central intensity of $2 \times 10^{14}$ s$^{-1}$sr$^{-1}$ [35].

The bright metastable neon beam is created using five laser cooling sections: a collimator, two transverse Doppler laser coolers, a Zeeman slower and a Magneto-optical compressor. A drawing of the Gemini atomic beam line is shown in Figure 3.2. All these laser cooling sections are described in detail in [35].

The laser light for all these cooling sections is supplied by a single ring dye laser, consisting of a Coherent 899 dye and an Innova 100 Argon-ion laser. The output power of the laser is typically 700 mW. The wavelength of the laser is stabilized one linewidth red-detuned from the Ne* $^3P_2 \leftrightarrow$ Ne** $^3D_3$ transition by using saturated absorption spectroscopy. The resulting linewidth of the laser is approximately 1 MHz. The laser frequencies needed for the different cooling sections are obtained using Acousto-Optic Modulators (AOM) [29].

The entire setup is situated in a vacuum system with a pressure ranging from $10^{-3}$ mbar at the source to $10^{-8}$ mbar after the Magneto-optical compressor (EMOC). In the trapping chamber the pressure is reduced to $\sim 10^{-9}$ mbar.

With every laser cooling section on the Gemini beam line can produce $5 \times 10^{10}$ atoms/s with a divergence of 3 mrad and an axial velocity of 100 m/s.
3.4.2 Trapping chamber

Figure 3.3 shows in detail the trapping chamber consisting of the MOT and the MT. The trapping chamber is separated from the Gemini beamline by an Edwards vacuum valve. Next a Stepper Motor controlled Ito-plate detector enables us to measure the atomic beam current and to align Gemini and the trapping chamber. The pressure is reduced by a factor 100 by two flow resistances. In addition, the pressure is maintained by an ion getter and a Ti-sublimation pump [9]. Theoretically, pressures of the order of $10^{-11}$ mbar, which are essential in reaching BEC, are now possible in the trapping chamber. The two large windows of the MOT perpendicular to the $z$-axis (§ 2.3), however, leak, because they can not be tightened enough. Both windows are pumped with a fore-vacuum pump. As a result the pressure in the trapping chamber is only $\sim 10^{-9}$ mbar.

Extra Zeeman slower

The capture velocity $v_c$ of the MOT is given by [1]:

$$v_c = \sqrt{(2ar)} = \sqrt{\frac{\hbar k T r}{2m}}, \quad (3.22)$$

and is equal to the velocity of an atom that is stopped in a distance equal to the radius $r$ of the trap by a force equal to half the maximum scattering force (3.4). For a typical value of $r = 2.9$ mm, this formula gives: $v_c = 48$ m/s. Since the atoms leave the Zeeman slower with an axial velocity of 100
Figure 3.4: The absolute value of the laser detuning $\delta_{\text{laser}}$, the Zeeman shift $\Delta \omega_Z$, and the Doppler shift $\omega_D$ as a function of the distance from the center of the MOT. Negative $y$-coordinates correspond to a position upstream from the center of the MOT. The laser detuning equals $\delta_{\text{laser}} = -6\Gamma$. The Zeeman shift is directly proportional to the magnetic field of the slower coils (3.5). The Doppler shift shown in the figure is the Doppler shift for atoms moving with an axial velocity of $v_0 = 100$ m/s. The atoms are resonant with the laser light of the slower beam when the sum of the Zeeman shift and the laser detuning is equal to the Doppler shift

$$\Delta \omega_Z + \delta_{\text{laser}} = \Delta \omega_D = \vec{k} \cdot \vec{v}_0.$$ 

Schematically the particle trajectory is depicted for atoms moving in a slower beam with, respectively, the right (path 1), a too strong (path 2) and a too low (path 3) intensity.

m/s, it is clear that the atoms need to be slowed further. A second Zeeman slower provides this extra slowing stage.

To keep the atoms resonant with the laser light over a velocity range, the atomic energy is shifted with an inhomogeneous magnetic field, so that the Doppler shift (depending on the changing velocity of the atom) is compensated by the Zeeman shift (depending on the magnitude of the magnetic field) (§ 3.2.2). Figure 3.4 shows the Zeeman, Doppler and laser detuning as a function of the distance from the center of the MOT. When the sum of the Zeeman shift and the laser detuning are equal to the Doppler shift $\Delta \omega_Z + \delta_{\text{laser}} = \Delta \omega_D = \vec{k} \cdot \vec{v}_0$, the atoms are resonant with the laser light and absorb photons. As a result the atoms are slowed down and their Doppler shift decreases. They travel further downstream until they are again resonant with the laser light. When the gradient of the slower field is chosen correctly, the atoms stay resonant with the laser beam and follow the curve of the Zeeman shift, until their velocity has become zero at the center of the trap, path 1.

In order to slow the atoms to velocities below the capture velocity of the MOT, it is very important that the intensity of the slowing beam is low enough. Because when the slowing laser beam has an intensity of $s_0 \approx 1$, also non-resonant photons are absorbed, and the atoms never reach the center of the trap, path 2. On the other hand, when the laser intensity is too low, the atoms absorb too few photons and will not follow the curve of the Zeeman shift. They reach the center of the trap with a relatively high velocity, or are not even slowed down enough to be captured by the MOT, path 3.

The extra Zeeman slower consists of 1 coil with 100 turns and a diameter of 80 mm at a distance...
of 120 mm upstream from the center of the MOT, and a second coil with 50 turns and a diameter of 300 mm at a distance of 190 mm downstream from the center of the MOT (Figure 3.3). Both coils are perpendicular to the beam- or y-axis and carry equal and opposed currents. These slower coils generate a spherical quadrupole field that is zero at the center of the MOT and has a maximum field strength of 100 G for \( I = 6 \) A. In combination with a circularly polarized laser beam, the atoms are slowed to velocities below the capture velocity, without disturbing the magnetic field of the MOT. The extra slower beam is red-detuned over \( \delta_{\text{Zeeman},2} = -6 \Gamma = -50(2\pi) \) MHz and has an intensity of 1 mW cm\(^{-2}\) or \( s_0 = 0.25 \).

**MOT**

The laser light for the MOT beams is supplied by a single dye laser, consisting of a Spectra Physics 380D dye laser, pumped by a 5 W Coherent Innova 70 Argon-ion laser. The output power of this laser is typically 300 mW.

The MOT consists of three orthogonal pairs of red-detuned, counter propagating, circularly polarized laser beams and a pair of coils with equal, opposed currents (subsection 1.4.1). The laser beams enter the trapping chamber under an angle of \(+45^\circ\) and \(-45^\circ\) with respect to the x-axis from above, and along the z-axis, respectively (Figure 3.3). These three laser beams are retroreflected to obtain three pairs of counterpropagating laser beams. The polarization of the reflected beams is changed from \( \sigma^+ \) to \( \sigma^- \) or vice versa, using a quarter wave plate.

The intensity of the retroreflected \( 45^\circ \) MOT beams is reduced, since the trapped atoms in the MOT attenuate the incoming laser beams. An intensity imbalance is the result. Due to this intensity imbalance, the atom cloud is shifted somewhat below the center of the MOT. An imbalance of \( \sim 10\% \) can only cause a displacement of the order of 1 mm. Our MOT is, however, shifted a few mm below the center, so an intensity imbalance alone is not enough to explain this shift.

Also the slower beam, coming from the \(+y\) direction, introduces an imbalance: the atom cloud is pushed in the \(-y\) direction. These intensity imbalances need to be compensated for each different setting of the intensity of the MOT and Zeeman slower laser beams.

The earth’s magnetic field and this intensity imbalance are compensated by three pairs of Helmholtz coils. These coils are wrapped around the trapping chamber and are indicated in Figure 3.3. In table 3.2 the coil parameters are listed.

Beside the Ito plate, three other detectors are available: a photo diode, a channeltron and a CCD camera. Both the photo diode and the CCD camera are located under the trapping chamber (Figure 2.4). A beam splitter directs half of the light towards the photo diode and half of the light towards the CCD camera. The channeltron is attached to the upper port of the trapping chamber (Figure 3.3).

In our setup we use a Galilei channeltron, which is operated at typically \(-3\) kV and has a gain of \( \sim 10^9 \). In front of the channeltron a nickel raster with a diameter of 10 mm is placed. By changing the voltage on this raster, the channeltron can be used to detect both ions and UV-photons and metastable neon atoms. When the voltage on the raster is negative (\(-200\) V) the positive neon ions are attracted and detected. When a positive voltage is applied to the raster (\(+200\) V), the neon ions are repelled, and UV-photons and metastables are detected. The opening angle and the detecting efficiency of both the channeltron and the photo diode are given in Table 3.3. The photo diode is used
Table 3.2: The geometry of the compensation coils. The shape of the coils, the size, the distance $2A$ between the coils, the number of turns and the magnetic field are given for the coils that compensate the earth's magnetic field and the intensity imbalance of the MOT and slower beams.

<table>
<thead>
<tr>
<th>Coil</th>
<th>Shape</th>
<th>Diameter (mm)</th>
<th>A (mm)</th>
<th>Turns</th>
<th>$B_0$ (G/A)</th>
</tr>
</thead>
<tbody>
<tr>
<td>I</td>
<td>round</td>
<td>250</td>
<td>89</td>
<td>75</td>
<td>4.19&lt;sup&gt;a&lt;/sup&gt;</td>
</tr>
<tr>
<td>II</td>
<td>round</td>
<td>432</td>
<td>108</td>
<td>100</td>
<td>4.16&lt;sup&gt;b&lt;/sup&gt;</td>
</tr>
<tr>
<td>III</td>
<td>square</td>
<td>372&lt;sup&gt;c&lt;/sup&gt;</td>
<td>146</td>
<td>100</td>
<td>3.29&lt;sup&gt;b&lt;/sup&gt;</td>
</tr>
</tbody>
</table>

<sup>a</sup> Measured value, calculations yield 4.076 G/A.
<sup>b</sup> Calculated values.
<sup>c</sup> Length of the square.

to do fluorescence spectroscopy. The CCD camera is used to image the trapped atom cloud. A second camera along the $z$–axis is used for absorption imaging.

3.5 Measurement techniques

In our experimental setup three measurement techniques can be used, which provide a measure for the number of particles in the trap: fluorescence spectroscopy, UV-photon decay and absorption imaging. Both the fluorescence intensity and the UV-photon decay of the atom cloud are directly proportional to the number of atoms in the trap. Absorption imaging can not only be used to determine the number of trapped particles, but can also be used to determine the velocity and temperature of the atom cloud.

Unfortunately, in our MOT it is not possible to measure UV-photon decay because the effective loss rate for this process is of the same order as the effective loss rate, due to collisions with the background gas (resulting in loss of metastable atoms), at the pressures currently obtainable in our MOT. Our channeltron can not distinguish between metastable atoms and UV-photons. Therefore, if we want to measure UV-photon decay, the effective decay rate for this process must be at least an order of magnitude larger than the loss rate due to background collisions. In this section the remaining two measurement methods are briefly described.

3.5.1 Fluorescence spectroscopy

A relatively quick and easy way to measure real time the number of atoms in the trap is fluorescence spectroscopy. A laser beam, either the MOT beams or a probe laser beam, is absorbed by the trapped atoms, which spontaneously decay while sending out a photon. In the measurements presented in the next section, the MOT beams are used to induce fluorescence. A telescope focuses the reemitted light on a photo diode. The fluorescence intensity is directly proportional to the number of atoms in the trap:

$$ I_{fluor} = N \Gamma_{scat} \left( \frac{\Omega}{4\pi} \right)_{det} \eta_{det} $$

(3.23)
Here $N$ is the number of trapped particles, $(\Omega/4\pi)_{\text{det}}$ the opening angle of the detector assembly, $T_{\text{lense}}$ the transmission of the focusing lenses, $\eta_{\text{det}}$ the detecting efficiency of the photo diode and $\Gamma_{\text{scat}}$ the scattering rate defined by [36]:

$$\Gamma_{\text{scat}} = \frac{\Gamma}{2} \frac{CS_{\text{tot}}}{1 + CS_{\text{tot}} + 4 (\frac{\delta}{\Gamma})^2}.$$  

(3.24)

Here $\delta = \omega - \omega_0$, which is equal to the detuning of the MOT beams at the center of the trap (both the Doppler shift and the Zeeman shift are negligible at the center of the trap). Furthermore, $\Gamma$ is the line width of the cooling transition and $S_{\text{tot}}$ is the intensity of all MOT laser beams combined divided by the saturation intensity $I_0$. The parameter $C$ is the effective Clebsh-Gordon coefficient of the $^3P_2 \rightarrow ^3D_3$ transitions and is determined experimentally $C \approx 0.7$ [36]. All relevant measurement parameters are given in Table 3.3.

### 3.5.2 Absorption imaging

**Introduction**

Absorption imaging can be used to measure the density and velocity distribution simultaneously. A probe beam that passes through the MOT impinges on a CCD camera. The probe diameter $d_p = 20$ mm, is much larger than the trap size ($l = 5.8$ mm), therefore absorption of the probe beam by the trapped atoms is visible as a shadow in the spatial profile of the probe beam intensity. This shadow is focused onto the CCD camera.

When taking absorption images at different delay times after the MOT has been turned off, the velocity distribution can be determined from the increase in radius of the atom cloud (the shadow in the absorption image) and the time elapsed between subsequent measurements. The temperatures along orthogonal directions can be obtained, assuming that the velocity distribution is Gaussian. The delay times must be short enough that the atoms do not leave the illuminated area.

First an absorption image is taken with an empty MOT, in order to supply a reference image. Then an absorption measurement with a loaded MOT is taken. The ratio of both these measurements yields a spatial profile of the probe beam attenuation, which is related to the spatial profile of the MOT density integrated along the probe beam direction.

**Image analysis**

Attenuation of a probe beam propagating along the $z$-axis (Figure 3.3) by the laser-cooled atom cloud in the MOT is assumed to satisfy Beer's law [39]:

$$I(x, y, z) = I(-\infty) \exp \left( -\sigma_a \int_{-\infty}^{z} n(x, y, z') dz' \right),$$  

(3.25)

where $\sigma_a$ is the absorption cross section and $n(x, y, z)$ the spatial density distribution of the the atoms in the MOT.

The trap density is assumed to be a three-dimensional Gaussian:

$$n(x, y, z) = n_0 \exp \left( -\frac{x^2}{2\rho_x^2} - \frac{y^2}{2\rho_y^2} - \frac{z^2}{2\rho_z^2} \right),$$  

(3.26)
where \( \rho_x, \rho_y \) and \( \rho_z \) are the rms radius along, respectively, the \( x- \), \( y- \) and \( z- \)axis, and \( n_0 \) is the maximum density given by:

\[
n_0 = \frac{N}{(2\pi)^{3/2}\rho_x\rho_y\rho_z}.
\] (3.27)

The optical density \( OD \) is defined as [39]:

\[
OD(x, y) = -\ln \left( \frac{I(x, y, \infty)}{I(x, y, -\infty)} \right).
\] (3.28)

Combining equation (3.25), (3.26) and (3.28) we obtain:

\[
OD(x, y) = \sigma_a \rho_z \sqrt{2\pi} n(x, y, 0).
\] (3.29)

The right hand side of equation (3.28) is equal to the ratio of the absorption and reference images and is used to obtain an experimental \( x, y \) profile of the density. The results are fitted with the product of one-dimensional Gaussians along the \( x \) and \( y \) direction. These fits yield \( \rho_z \), \( \rho_y \) and the maximum optical density. Since the axial magnetic field gradient of the MOT quadrupole field is twice as big as the radial magnetic field gradient (A.9), \( \rho_z \) in equation (3.29) may be replaced by \( \rho_x/2 \), which is obtained from the above mentioned fit. The maximum density is then equal to:

\[
n_0 = \frac{-\ln \left( \frac{I(0,0,\infty)}{I(0,0,-\infty)} \right)}{\sqrt{2\pi} \sigma_a \rho_x/2}.
\] (3.30)

The absorption cross section \( \sigma_a \) can be calculated using equation (3.18). The spatial density distribution is then obtained from equation (3.26) and (3.30).

The velocity distribution is determined by comparing absorption images at different delay times, \( t_1 \) and \( t_2 \). Assuming the velocity distribution to be Gaussian, a rms velocity can be obtained along both the \( x- \) and \( y- \)axis. Comparing two absorption images, taken after different delay times, the measured rms radius along both the \( x- \) and \( y- \)axis (e.g. \( \rho_x \) and \( \rho_y \)) is given by:

\[
\rho^2(t_2) = \rho^2(t_1) + v_{xi}^2(t_2 - t_1)^2,
\] (3.31)

where \( \rho(t_1) \) is the rms radius of the atom cloud after a delay time of \( t_1 \) s and \( v_{xi} \) the rms velocity along the \( x_i = x \) or \( y \) axis. Since \( \rho_x(t_1), \rho_x(t_2), \rho_y(t_1) \) and \( \rho_y(t_2) \) are measured, both \( v_x \) and \( v_y \) can be obtained straightforwardly from equation (3.31).

The one dimensional temperature in its turn can be obtained from the following relation:

\[
T_{x_i} = \frac{mv_{xi}^2}{k_B},
\] (3.32)

where \( x_i \) is either \( x \) or \( y \).

**Example**

Because the number of atoms lost from the trap due to ionization is proportional to the square of the particle density, a large \( (V \approx 0.1 \text{ cm}^3) \) so-called Hard Sphere MOT is used to minimize trap losses.
3.6 MEASUREMENTS

Such a MOT can be obtained when using laser beams with low laser power $I = 0.5 I_0$, and a large negative detuning $\delta = -5\Gamma$, combined with a moderate magnetic field gradient of $\sim 1 \text{ G/mm}$ [34, 20].

For a circularly polarized probe laser beam with detuning $\delta = -5\Gamma$, impinging on a Ne* MOT with initial conditions $T = 250 \mu\text{K}$, $N = 10^{10}$ atoms and $n_0 = 10^{11} \text{ cm}^{-3}$, the absorption cross section is equal to $\sigma_a(\delta = -5\Gamma) = 1.94 \times 10^{-15} \text{ m}^2$. From equation (3.29) we now obtain an optical density of $OD = 0.7$, assuming $\rho_x/2 = l/4 = 1.45 \times 10^{-3} \text{ m}$. At resonance ($\delta = 0$) the optical density is a factor 100 higher. At low optical densities, detecting the ratio between the intensities of the absorption and reference image becomes a problem.

The force exerted by the probe laser beam on the atom cloud is equal to the constant scattering force exerted by a running wave (3.1). For a circularly polarized probe laser beam with a detuning of $\delta = -5\Gamma$, and a saturation parameter $s_0 = 0.5$, the scattering force at the center of the trap is equal to $-8.88 \times 10^{-21} \text{ N}$, corresponding to an acceleration of $a = -2.68 \times 10^5 \text{ ms}^{-2}$. The time it takes to displace an atom with either 1, 2 or 5 mm is then equal to 61, 86 and 137 $\text{ ms}$, respectively. Therefore, to avoid large displacements of the atom cloud, the probe beam should only be switched on for short pulses $\Delta t < 60 \mu\text{s}$.

In order to be able to do absorption imaging the radius of the probe laser beam should at all times be greater than the rms radius $\rho$ of the (expanding) atom cloud. In our case the maximum diameter of the probe laser beam is 20 mm, limited by the size of the windows of the trap. This corresponds to a rms radius of 8.5 mm. Thus the radius of the atom cloud should be smaller than 8.5 mm. Using equation (3.31) and assuming $\rho_{0x} = \rho_{0y} = 2.9 \text{ mm}$ and $T = 250 \mu\text{K}$, we then obtain $\tau < 25 \text{ ms}$. Or in other words, 25 ms after turning off the MOT, the atom cloud will have the same size as the probe laser beam and absorption imaging is not feasible anymore.

At $T = 250 \mu\text{K}$ and $\Delta t > 9 \text{ ms}$, the rms radius of the cloud in the $x$ and $y$ direction, increases linearly with time. The expansion velocity $v_c$ is then constant and equal to: $v_c = 0.32 \text{ ms}^{-1}$.

3.6 Measurements

In order to realize BEC, the number of particles in the MOT must be optimized. In addition, the lifetime of the MOT must be greater than the time needed to transfer the atoms from the MOT to the MT. Also, we want to cool the atoms in the MOT to as low as possible temperatures. Therefore, in this section, first measurements on optimization of the MOT are presented.

The loss of atoms from the MOT or trap decay, after switching off the loading beam, has been measured as a function of the detuning of the MOT laser beams for different MOT magnetic field gradients. During one second the MOT is loaded, then the loading is stopped for one second, by switching off all the laser cooling sections of the Gemini beamline, and the process is repeated. All five cooling sections of the Gemini beamline are disabled with a mechanical shutter, during the decay stage. Two decay cycles, which show the fluorescence as a function of the time, are depicted in Figure 3.5. The MOT is left turned on during the decay. The fluorescence is induced by the MOT beams.

In § 3.3 we have seen that $\tau_{gas} \gg \tau_{ion} \sim 0.1 \text{ s}$, therefore our loss rate is dominated by ionization and we can neglect the loss rate $\kappa_{gas} \cdot n_{gas}$ due to collisions with the background gas. At lower MOT densities the loss rate due to collisions with the background gas become dominant.

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Figure 3.5: Two fluorescence decay cycles of the MOT. The figure shows the fluorescence signal of the photo diode in nA, as a function of time. At $t = -1$ and $t = 1$ s, the MOT is loaded for 1 s. After 1 s, at $t = 0$ and $t = 2$, the loading is stopped for 1 s.

The solution to equation (3.21), when neglecting collisions with the background gas, is:

$$N(t) = \frac{N_0}{1 + (t - t_0)/\tau_{\text{ion}}},$$  

(3.33)

where

$$\tau_{\text{ion}} = \frac{1}{\beta_{\text{ion}}n_0},$$  

(3.34)

with $\beta_{\text{ion}}$ the ionization rate constant, $n_0$ the particle density at the center of the trap and $t_0$ the time at which the decay starts.

The decay curves of the MOT are fitted with equation (3.33), using a least squares program. These fits yield the number of particles in the MOT $N_0$ and the time constant $\tau_{\text{ion}}$ for loss due to ionization. One fluorescence decay curve and its fit are given in Figure 3.6, for a MOT magnetic field gradient of $B' = 1$ G/mm, a detuning of the MOT beams of $\delta = 2.77\Gamma$ and a saturation parameter of $S_{\text{tot}} = 7$. Here $S_{\text{tot}}$ is the saturation parameter of all six MOT laser beams combined. The time constant for ionization or the lifetime of the trap is for these MOT parameters equal to $\tau_{\text{ion}} = (0.025 \pm 0.002)$ s.

The steady state volume of the confined atom cloud is determined in the following way. First, every 20 ms, a picture of the MOT is taken with the CCD camera. The rms long $\rho_y$ and short axis $\rho_z$ of the elliptical cloud are determined for each picture using a Gaussian fit. The volume of the MOT, is then equal to [25]:

$$V = (2\pi)^{3/2}\rho_y^2\rho_z.$$  

(3.35)
The volume of the MOT decreases when more and more atoms are lost from the trap. The steady state volume of the MOT (the equilibrium volume of the MOT with the loading beam switched on) gives, however, in good approximation the volume of the MOT during the decay, since the time constant for loss due to ionization is determined by the first steep part of the decay curve, when the volume of the MOT is still approximately constant.

The number of particles \( N \) in the MOT, the volume \( V \) of the confined atom cloud, the particle density \( n \) in the MOT, the time constant \( \tau_{\text{ion}} \) for loss due to ionization and the ionization rate constant \( \beta_{\text{ion}} \) are determined from the fluorescence spectra as a function of the detuning of the MOT laser beams, for different MOT magnetic field gradients. Table E.1 in Appendix E summarizes the results.

The uncertainty in the fit is indicated for all measurements. There may be a systematic error of the order of 10% in the scattering rate \( \Gamma_{\text{scat}} \) (3.24), which causes a systematic error in the number of a particles \( N \), the particle density \( n_0 \) and the ionization rate constant \( \beta_{\text{ion}} \). This systematic error in \( \Gamma_{\text{scat}} \) is mostly due to the systematic error in the laser detuning \( \Delta \delta = 2 \text{ MHz} = 0.24 \Gamma \). The average total uncertainty (including the uncertainty in the fit) in the number of particles, the particle density and the ionization rate constant, are respectively equal to 20%, 35% and 50%.

The number of particles in the MOT is determined from the fluorescence intensity, using equation (3.23) and (3.24). Figure 3.7 shows the number of trapped particles in the MOT as a function of the laser detuning \( \delta \), for a low \( B' = 0.25 \text{ G/mm} \) and a high gradient \( B' = 1.8 \text{ G/mm} \) of the MOT magnetic field.

The laser detuning for which the number of particles in the MOT is maximum increases when the magnetic field gradient of the MOT increases. This is what we expect, since the balance between the Zeeman shift and the laser detuning determines the volume of the MOT. However, this relationship

---

Figure 3.6: Fluorescence decay curve of the number of particles in the MOT as a function of time, for \( B' = 1 \text{ G/mm} \). The time constant of the decay is \( \tau_{\text{ion}} = (0.025 \pm 0.002) \text{ s} \).
Figure 3.7: Number of trapped particles in the MOT as a function of the laser detuning $\delta$, for a low and high gradient $B'$ of the MOT magnetic field. The maximum number of particles in the MOT does not seem to increase for lower magnetic field gradients.

between the MOT magnetic field gradient $B'$ and the laser detuning $\delta$ is clearly not linear. From the resonance condition $\delta_{\text{laser}} = \Delta \omega Z \propto B' \rho_z$, we expect a linear relationship between $B' \rho_z$ and $\delta$.

We expect an increase in the total number of trapped particles in the MOT for lower magnetic field gradients, because, for lower magnetic field gradients, the volume of the MOT is larger and thus more particles could be trapped in the MOT. However, the maximum number of particles does not increase for lower magnetic field gradients, it stays more or less constant.

A possible explanation for this lack in increase of the number of particles in the MOT for smaller magnetic field gradients, could be a large optical density at small detunings. Figure 3.8 shows the optical density (3.29), calculated for a MOT magnetic field gradient of $B' = 1.0$ G/mm. The central density is in this case equal to $n_0 = 4.6 \times 10^{10}$ cm$^{-3}$ and the rms radius of the cloud is equal to $\rho_z = 0.42$ mm for a laser detuning of $\delta = 2.77\Gamma$. Figure 3.9 shows the corresponding transmission of the laser light. From these figures it is clear that, the optical density has no major influence on the measured number of particles, since the optical density is very small for detunings larger or equal to 2.77 $\Gamma$.

The reason why the absolute number of particles in the MOT is difficult the measure, using fluorescence spectroscopy, is that reradiated light by the atoms, the fluorescence, is always resonant. Therefore, the cross section for absorption of reradiated light $\sigma_R$ is larger than the cross section for absorption $\sigma_a$ of the laser light for non-zero laser detunings. As a result, the number of particles measured with fluorescence spectroscopy is lower than the actual number of trapped atoms in the MOT. Recent absorption imaging measurements seem to confirm this.

Figure 3.10 shows the volume of the trapped atom cloud in the MOT as a function of the detuning of the MOT laser beams, for a magnetic field gradient $B' = 1.0$ G/mm. The volume of the confined
Figure 3.8: Calculated optical density $\text{OD}$ as a function of the laser detuning. The optical density is calculated using equation (3.29) and $n_0 = 4.6 \times 10^{10}$ cm$^{-3}$ and $\rho_z = 0.42$ mm. These values have been measured for $B' = 1.0$ G/mm and $\delta = 2.77\Gamma$.

Figure 3.9: Calculated transmission of the laser light through the atom cloud, as a function of the laser detuning, for a MOT with magnetic field gradient $B' = 1.0$ G/mm and laser detuning $\delta = 2.77\Gamma$. The measured density and rms radius are, respectively, equal to $n_0 = 4.6 \times 10^{10}$ cm$^{-3}$ and $\rho_z = 0.42$ mm.
Magnetooptical Trap

Figure 3.10: Volume of the trapped atom cloud as a function of the detuning of the MOT laser beams, for a magnetic field gradient of $B' = 1 \text{ G/mm}$. The volume of the MOT increases with the detuning of the MOT beams cubed: $V \propto \delta^3$. The data has been fitted with $V = 1.7 \times 10^{-4}\delta^3$.

atoms in the MOT increases with the detuning of the MOT laser beams as $V \propto \delta^3$. This can be understood as follows. At the center of the MOT, the velocity of the particles is approximately zero and therefore, we can neglect the Doppler shift. The volume of the MOT is now determined by the balance between the Zeeman shift, due to the quadrupole field of the MOT, and the MOT laser detuning $\delta_{\text{laser}} = \Delta \omega_2 \propto B' \rho_z$ (3.5).

This is the case for all four MOT magnetic field gradients. However, the volume of the MOT does not change as a function of the magnetic field gradient, except at very low ($B' = 0.25 \text{ G/mm}$) gradients (Table E.1). This is in contradiction with the behaviour of the volume as $\propto \delta^3 = (\Delta \omega_2)^3 \propto B'^3$. We do not have an explanation for this.

Figure 3.11 shows the central particle density of the confined atoms in the MOT as a function of the MOT laser detuning, for $B' = 1 \text{ G/mm}$. The density is determined by dividing the number of particles in the MOT by the steady state volume. Generally the particle density in the MOT increases for larger gradients of the MOT magnetic field. This is according to expectations because a larger magnetic field gradient means a larger spring constant and thus a stronger confining force; the particles are more strongly compressed and the density increases. In addition, the density decreases as a function of the laser detuning, for all (measured) magnetic field gradients. Since, in general, a larger laser detuning and a smaller magnetic field gradient, result in a larger MOT volume, this is in agreement with expectations.

Figure 3.12 shows the loss rate due to ionization $\beta_{\text{ion}}$ as a function of the MOT laser detuning, for a MOT with $B' = 1.0 \text{ G/mm}$. The ionization loss rate constant due to ionization is approximately constant as a function of the laser detuning $\beta_{\text{ion}} = (9 \pm 2)10^{-10} \text{ cm}^3\text{s}^{-1}$.

The ionization rate constant is for all magnetic field gradients, of the order of $\beta_{\text{ion}} \approx 10^{-9} \text{ cm}^3\text{s}^{-1}$. These values are clearly larger than the ionization rate constant $\kappa_{\text{ion}} = 5 \times 10^{-11}$ calculated by

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Figure 3.11: Central particle density in the MOT as a function of the MOT laser detuning, for four different gradients of the MOT magnetic field, respectively, $B' = 0.25, 1.0, 1.8$ and $2.6$ G/mm.

Figure 3.12: Penning ionization loss rate $\beta$ as a function of the laser detuning for a MOT with $B' = 1$ G/mm. The loss rate due to ionization is approximately constant as a function of the laser detuning $\beta_{\text{ion}} = (9 \pm 2) \times 10^{-10}$ cm$^3$s$^{-1}$. 
Doery et al (1.7) [23]. The difference between these two ionization rate constants is, that the latter $\kappa_{ion}$, is the rate constant for ionization due to collisions between two Ne* (3s) atoms. In our MOT, however, we use the MOT beams to induce fluorescence. Therefore, light assisted collisions between Ne* (3s) and Ne** (3p) atoms ($s+p$-collisions) will also occur. As a result the ionization rate constant is an order of magnitude larger. Tol et al found for the loss rate of metastable triplet helium due to $s+p$-ionizing collisions $\beta_{3sp} \approx 5 \times 10^{-9} \text{ cm}^3 \text{s}^{-1}$ [25]. In the absence of light, losses are caused only by ionizing He* (3s) - He* (3s) ($s+s$)-collisions, and they found $\beta_{3ss} = (1.3 \pm 2) \times 10^{-10} \text{ cm}^3 \text{s}^{-1}$ [25]. These values are within a factor 2 (and thus within the measurement uncertainty) consistent with our measured ionization rate constant for light assisted collisions $\beta_{ion}$ and the calculated ionization rate constant $\kappa_{ion}$ (1.7) for Ne* (3s) - Ne* (3s) collisions.

In order to determine the ionization rate constant for Ne* (3s) - Ne* (3s) collisions as well as for light assisted Ne* (3s) - Ne** (3p) collisions, the decay of the MOT in the 'absence' of light should be measured, i.e. using a weak probe laser beam, instead of the MOT laser beam, for fluorescence spectroscopy.

The lifetime of the MOT, due to ionization, is approximately constant or increases slightly as a function of the laser detuning (Figure 3.12). The over the detuning averaged time constant for light assisted ionization is for a MOT gradient of, respectively, $B' = 0.25, 1.0, 1.8$ and $2.6 \text{ G/mm}$ equal to, respectively, $\tau_{ion} = 0.085, 0.051, 0.053$ and $0.039 \text{ s}$. These lifetimes are long enough to cool the atoms in the MOT to the origin ($\tau = 1.5 \text{ ms (3.14)})$ and to successively transfer them from the MOT to the MT ($\tau_{transfer} \sim 1 \text{ ms}$).

---

Table 3.3: Measurement parameters.

<table>
<thead>
<tr>
<th>Quantity</th>
<th>Symbol</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Opening angle photo diode</td>
<td>$\frac{\Pi}{4\pi}_{\text{photo}}$</td>
<td>$(7.6 \pm 0.3) \times 10^{-4} \text{ sr}^{-1}$</td>
</tr>
<tr>
<td>Detecting efficiency fluorescence</td>
<td>$T_{\text{fenseqdet}}$</td>
<td>$(3.9 \pm 0.2) \times 10^{-20} \text{ A photons/s}$</td>
</tr>
<tr>
<td>Total saturation parameter</td>
<td>$S_{\text{tot}}$</td>
<td>7.0</td>
</tr>
<tr>
<td>Effective Clebsch Gordon coefficient</td>
<td>$C^a$</td>
<td>$(0.7 \pm 0.2)$</td>
</tr>
<tr>
<td>Detuning</td>
<td>$\delta$</td>
<td>9.68</td>
</tr>
<tr>
<td>MOT Magnetic field gradient</td>
<td>$\nabla B$</td>
<td>0.033 $\text{ GA}^{-1}\text{mm}^{-1}$</td>
</tr>
<tr>
<td>Current coil I</td>
<td>$I$</td>
<td>0.00</td>
</tr>
<tr>
<td>Current coil II</td>
<td>$I$</td>
<td>$-0.11$</td>
</tr>
<tr>
<td>Current coil III</td>
<td>$I$</td>
<td>$+0.51$</td>
</tr>
<tr>
<td>Opening angle channeltron</td>
<td>$\frac{\Omega}{4\pi}_{\text{chan}}$</td>
<td>$(5.0 \pm 0.3) \times 10^{-3} \text{ sr}^{-1}$</td>
</tr>
<tr>
<td>Detecting efficiency channeltron for ions</td>
<td>$D_{\text{ion}}$</td>
<td>1.0</td>
</tr>
<tr>
<td>Detecting efficiency channeltron for UV-photons</td>
<td>$D_{\text{UV}}$</td>
<td>0.1</td>
</tr>
<tr>
<td>Detecting efficiency channeltron for metastables</td>
<td>$D_{\text{Ne}^*}$</td>
<td>1.0</td>
</tr>
</tbody>
</table>

[a][36]
3.7 Conclusions

We have at least observed $5 \times 10^8$ particles in our MOT. To further check the absolute number of trapped particles in the MOT, other measurement techniques, such as absorption imaging, could be applied. The particle density increases as a function of the magnetic field gradient and has a maximum value of $(6.6 \pm 0.9) \times 10^{10} \text{ cm}^{-3}$.

The observed light assisted ionization rate constant is of the order $\beta_{\text{ion}} \approx 10^{-9} \text{ cm}^3 \text{s}^{-1}$ and is consistent with measurements on triplet metastable helium [25].

The lifetime of the MOT, due to ionizing collisions, changes from $\tau_{\text{ion}} = 0.085$ to 0.039 s for, respectively, low and high MOT magnetic field gradients. This lifetime is, in all cases, enough to cool the atoms in the MOT to temperatures in the $10 \mu$K regime and to successively transfer them from the MOT to MT. However, to obtain the desired number of particles in the MOT, $N \sim 10^{10}$, and the desired MOT volume, $V \geq 0.1 \text{ cm}^3$, the MOT needs to be optimized further.
Chapter 4

Photo Association Spectroscopy

4.1 Introduction

As we have seen before, Bose Einstein Condensation occurs when the mean distance separating the atoms is of the same order as the De Broglie wavelength $\Lambda$. At the low temperatures necessary to achieve the critical phase space density, the collision time becomes several times the spontaneous emission lifetime $\tau$, and the inhomogeneous Doppler line width becomes smaller than the natural width of the atomic dipole transition. As a result, two interacting atoms have plenty of time during a collision, to absorb energy from an external radiation field or emit energy by spontaneous or stimulated emission processes. Using this feature of ultra cold collisions, photo-association spectroscopy can be used for high precision measurements of collision parameters. Photo-association occurs when two free atoms absorb a photon and couple to an excited bound molecular state. This process will be explained in more detail in the next section.

In a condensate, collisions are characterized by an asymptotic phase shift $\eta_l$ or scattering length $a$ of the ground state wave function. This scattering length $a$ is defined as the effective point of origin of the long-range asymptotic ground state wavefunction, since this wave function is proportional to $\sin(k (r - a) - \frac{\pi}{2} l) = \sin(k r - \frac{\pi}{2} l + \eta_l)$. Here $k$ is the wavenumber, $r$ the interatomic separation between the atoms and $l$ the orbital angular momentum. The scattering length is given by [16]:

$$a = - \lim_{k \to 0} \left( \frac{\tan \eta_l}{k} \right).$$

(4.1)

Its sign determines whether a Bose Einstein condensate will be stable or unstable. A positive scattering length means a stable condensate, because in that case the atoms repel each other. A negative scattering length, however, results in an unstable condensate, because then the interaction between the atoms is attractive. The condensate collapses if, at a certain (negative) value of the scattering length, a critical number of atoms has been trapped [27].

In addition, the evaporative cooling rate necessary to obtain a BEC depends on the elastic scattering cross section $\sigma_{el} = 8\pi a^2$. The main purpose of the calculations in this chapter and future photo-association spectroscopy (PAS) measurements is, therefore, to determine the scattering length of metastable neon.

The scattering length is very sensitive to small changes in the short range interatomic potential. The short range interatomic potential of metastable neon is, however, not known. The short range
Na$_2$ X$^3\Sigma_u^+$ and Na$_2$ A$^3\Pi_u$ potentials [8], which are an approximation of the Ne$^*$-Ne$^*$ ground state and Ne$^*$-Ne$^{**}$ excited state potential, respectively, are usually used as input parameters in calculations. The molecular states are given in Hunds case (a) notation $\Lambda_{u/g}$, where $\Lambda$ is the projection of the orbital angular momentum on the molecular axis, denoted by either $\Sigma$, $\Pi$ and $\Delta$, for $\Lambda = 0, 1, 2$, respectively [41]. The correlation between the lab-fixed frame and the molecule-fixed frame is given in Appendix F. This is the correct notation at small internuclear separation when the coupling to the internuclear axis is stronger than the spin-orbit interaction and the rotation of the molecule is small. The indices $u$ and $g$ give the parity of the state and indicate, respectively, odd and even symmetry.

The short-range potentials of Na$_2$ can be used to approximate the Ne$^*$ - Ne$^*$ and Ne$^*$ - Ne$^{**}$ potentials, because the valence electronic structure of a singly excited rare gas atom is equal to that of a ground state alkali atom. The difference between ground state Na and metastable Ne$^*$ is the 2p core hole in the latter.

Only very recently, Kotochigova et al [28] have determined the short range Ne$_2$ 4$\sigma$ and 5$\pi$ potentials, using ab initio calculations. In this report, for the first time real neon potentials are used as input parameters, instead of the sodium potentials. The molecular potential curves are labeled by Hund's case (c) notation $\Omega_{g/u}$, where $\Omega$ is the projection of the total angular momentum on the internuclear axis. This is the correct notation for heavy nuclei at large internuclear separation with a strong spin-orbit interaction. The total angular momentum couples to the internuclear axis to make the projection $\Omega$. The orientation of the molecule-fixed frame as well as the vector diagram of Hund's case (c) coupling are given in Appendix F.

The non-relativistic ab initio electronic potentials are calculated using a multi-configuration valence-bond method [28]. However, no calculated potential is accurate enough to predict the scattering length. Fortunately, the effect of the short-range potential can be represented by its phase integral, which is defined as [23]:

$$\phi = \int_{r_{in}}^{r_0} k(r) dr = \int_{r_{in}}^{r_0} \frac{\sqrt{2\mu(E - V(r))}}{\hbar} dr,$$

(4.2)

where $r_{in}$ and $r_0$ are, respectively, the classical inner and outer turning point for a ground state atom with kinetic energy $E$ and $V(r)$ is the potential under consideration. When the phase integral of the ground state molecular potential is decreased by $\pi$, the potential well will support one bound vibrational level less. The scattering length will then first go to $-\infty$ and then change to $\infty$, or the other way around. These singularities occur at a zero energy resonance, or when the potential is almost not strong enough anymore to support the upper bound vibrational level.

Because we do not know the exact behaviour of the ground state potential, we do not know the exact value of the phase integral. To study the influence of the precise value of the phase integral on the scattering length, we can add to the ground state molecular potential a Gaussian 'bump' in such a way that its phase integral can be changed by $[0, \pi]$, by varying the height of the bump. For each of these potentials the photo-association spectrum and the scattering length are calculated. In this way we obtain a "fingerprint" of the loss rate due to photo-association as a function of the scattering length. Comparing future measurements with this "fingerprint" will hopefully yield the scattering length and the phase integral of the ground state interatomic potential.

If the scattering length of $^{20}$Ne$^*$ proves to be negative, its isotope $^{22}$Ne$^*$, might prove to have a positive scattering length. Therefore, also the scattering length of $^{22}$Ne$^*$ is calculated as a function of the phase integral of its molecular ground state potential.
This chapter is organized as follows. First the principle of photo-association is explained in § 4.2. Second, the differences between rare gas atoms and alkali-metal atom with respect to photo-association are discussed in § 4.3. Third, an analytical expression for the photo-association spectrum is given in § 4.4. Special attention is given to the transition rate from the free ground state to the bound molecular vibrational excited state in § 4.5. In § 4.6 the calculation are presented. Finally, some conclusions are presented in § 4.7.

4.2 Photo-association

Photo-association (PA) occurs whenever a colliding pair of atoms absorbs a photon and then couples to a bound excited molecular state. Figure 4.1 depicts the process. When the photon energy $\hbar \omega_L$ of a tunable laser matches the energy difference $E_v - E_g$ between an excited bound vibrational level $v$ and the asymptotic ground state $g$, a laser photon will be absorbed and the two atoms will couple into a molecular bound vibrational state. The transition rate for this process is given by $\gamma_{\ell} / h$. The laser frequency is equal to $\omega_L = \omega_0 - \delta_v - \delta_0$. Here $\hbar \omega_0$ is the energy difference between the ground and excited state in the asymptotic limit, $\delta_v$ the detuning of the laser relative to the bound vibrational state $v$, and $\hbar \delta_0$ the energy of the bound vibrational state relative to the asymptotic or dissociation energy of the excited state.

At a certain distance $R_C$ between the two colliding atoms, the laser frequency $\omega_L$ will become resonant with the transition to the excited bound state. At this so-called Condon radius, the original pair of colliding atoms can make an electric dipole transition to the molecular bound vibrational state. The Condon radius is defined by: $U_e(R_C) - U_g(R_C) = \hbar \omega_L$, where $U_e$ and $U_g$ are respectively the excited and ground state interaction potentials.

If the excited bound level decays to a product state $p$, which is detected as a function of the laser photon energy $\hbar \omega_L$, the resulting spectrum can be used to determine the positions of the excited bound state levels [16]. In a trap, this radiative escape process can be an important source of loss if each atom receives enough kinetic energy to overcome the trapping forces. The spontaneous decay of the excited bound state to the ground state by emission of a photon will generally lead to the loss of the two atoms from the trap, since the kinetic energy which they gain in the excited state potential well, $\Delta E \sim 1000$ K, exceeds the trap depth $\mathcal{E} \sim 1 - 5$ mK greatly.

There are two major contributions to the transition probability from ground to excited state. First, according to the Franck-Condon principle, the kinetic energy $\varepsilon$ and the position of the particles need to be conserved classically before and after the transition. So, when the kinetic energy and thus the local De Broglie wavelength of the ground and excited state wave functions match, the transition probability is maximum. However, because of the uncertainty principle other transitions can also occur.

Second, the transition probability is maximum at the turning points of the excited state potential, where almost all kinetic energy of the atoms is converted into potential energy and the atoms spend consequently most of their time. This transition probability is proportional to the square of the bound-free Franck-Condon integral. The Franck-Condon integral describes the overlap between the ground state $|g, \varepsilon\rangle$ and excited state $|e, v\rangle$ wave functions and is defined as: $\int \langle g, \varepsilon | e, v \rangle d\mathbf{r}$. For cold collisions, only the range of $\tau$ closely surrounding the outer turning point of the excited state potential contributes to the overlap between the ground and excited wave functions.
Figure 4.1: Diagram of the photo-association process. The potential curves of the ground $U_g$ and excited state $U_e$ are drawn as a function of the distance $r$ between two colliding atoms. These two colliding atom will be excited to a bound molecular state $v$, if the photon energy $\hbar \omega_L$ of a tunable laser, matches the energy difference $E_v - E_g = \hbar \omega_L$ between an excited bound level $v$ and the asymptotic free ground state $g$. Here $E_g$ is the energy of the original ground state and $E_v$ the energy of the excited bound state. The transition rate for this process is given by $\gamma_t / \hbar$. The laser frequency is equal to $\omega_L = \omega_0 - \delta_v - \delta_0$. Here $\hbar \omega_0$ is the energy difference between the ground and excited state in the asymptotic limit, $\delta_v$ the detuning of the laser relative to the bound vibrational state $v$ and $\delta_0$ the detuning of the bound vibrational state relative to the asymptotic or dissociation energy of the excited state. Second, this excitation will be followed either by spontaneous or stimulated emission back to the continuum levels of the ground state with decay rate $\gamma_s / \hbar$ or by decay to a product state $p$. The total decay rate is equal to $\gamma_p / \hbar$. All these processes generally result in the loss of atoms from the trap, because the energy the atoms gain $\Delta E$ in the excited state potential well exceeds the trap depth.
The excited quasi-bound molecule may also decay around the inner turning point of the excited state potential to bound levels of the ground molecular state. The probability for this transition is, however, small, since the potential is very steep around the inner turning point. Therefore, the atoms will spend far less time around the inner turning point than around the outer turning point. In addition, the overlap between the ground and excited state potential is small near the inner turning point, because the wave functions oscillate rapidly in this regime. This is also the reason why the long-range attractive potentials are dominant in the cold and ultra cold photo association process. In addition, Ne* atoms can auto-ionize, thereby gaining kinetic energy. The ions produced can be detected with high efficiency using a channeltron.

In our future PAS experiment the atoms are first loaded into the MOT during one second. After they have been cooled to temperatures around the sub-Doppler limit they are transferred from the MOT to the MT. The atomic density is about $10^{11}$ cm$^{-3}$ and the temperature is $\sim 250 \mu$K (the atoms gain potential energy during the transfer). After the transfer to the MT the atoms are spin-polarized.

Once the MT has been loaded, a right hand circularly polarized $\sigma^+$ PA probe laser beam with frequency $\omega_L$ is applied for $\sim 100$ ms, inducing loss of atoms. The metastable atoms lost from the trap are detected using a channeltron. Another possibility is to measure the number of atoms in the trap with laser-induced fluorescence, using a second probe beam. This process is repeated for a number of PA probe laser beam frequencies $\omega_L$.

While scanning the laser frequency $\omega_L$, trap losses will increase when the laser frequency is tuned to a photo-associative resonance. Using fluorescence spectroscopy or a channeltron, the loss of atoms, and thus the number of excited atoms, can be determined, as a function of the scanning laser frequency or the detuning of the laser from a vibrational bound state resonance $\delta_v$. The fluorescence intensity will sharply decrease, and the signal of the channeltron sharply increase, when the laser is tuned to a free-bound resonance.

In this way Photo-association Spectroscopy (PAS) can be used to determine the energies of the bound excited states of an atom. From the line shapes and intensity of these photo-associative spectra detailed information on the potential and scattering wave function can be obtained. Thus, experimental PA spectra combined with theoretical analysis could yield an accurate description of the scattering length and other collision properties relevant for achieving BEC. In addition detailed information on the long-range interactions of collision systems in the ground- and photo-excited states can be obtained.

Photo-association spectra display so-called Frank-Condon oscillations [38]. Since the transition amplitude from the 'ground' state $g$ to the excited bound state $v$ is directly proportional to the product of the respective wave functions, the Franck-Condon integral, and only the overlap in a range of $r$ closely surrounding the outer turning point of the excited state potential contributes to the Franck-Condon integral, nodes in the 'ground' state wave functions generate minima in the photo-association spectrum. The position of these 'ground' state wave function nodes can be determined from the Frank-Condon oscillations, supplying extra information on the 'ground' state wave functions and potentials.

Photo Association Spectroscopy can also be used to do precision measurements of vibration-rotation progressions from which accurate excited-state potential parameters can be determined. In addition, analysis of line profile measurements yields collision temperature and threshold behaviour or gives information about loss processes like ionization.

When the two atoms are sufficiently separated so that that their electron distributions do not
overlap, the interaction between them can be expressed in a multipole expansion. At long range electrostatic dispersion forces give rise to the ground state molecular potential varying as an attractive induced dipole interaction of the form $\frac{C}{r^6}$. Since the two atoms are homonuclear, the excited molecular interaction potential is an attractive resonant dipole interaction of the form $\frac{C}{r^3}$. The quadrupole-quadrupole interaction with behaviour $U_{q-q} \propto C_3/r^5$ is small compared to the $\propto r^{-3}$ and $\propto r^{-6}$ contributions to the interaction potential [22].

The vibration progressions can be determined from the fluorescence spectrum by plotting the bound vibrational energies (the laser frequencies where the fluorescence intensity shows a dip) as a function of the vibrational quantum number $v$. This relation yields the $C_3$ coefficient, since $\frac{\partial E_v}{\partial v} \propto C_3^{-1/3}$. Because each state characterized by $\Omega$, has its own characteristic $C_3$ coefficient at long range, the vibration progression can now be determined.

4.3 Rare gas versus alkali-metal atoms

In this chapter the photo-association of Ne*-Ne* into Ne*-Ne** is studied. Photo-association of metastable rare gas atoms like Ne* is different from photo-association of alkali-metal atoms, because the metastable Ne* atoms are, to start with, already in an excited state. In rare gas atoms, the Spin-Orbit (SO) interaction, which is absent in ground-state alkali systems, should be taken into account. In addition the high internal electronic energy of the rare gas atoms ensures that Penning ionization at small internuclear distances results in loss of atoms [24].

The rare gas atoms differ also from the alkalis in that respect that the most abundant isotopes have total nuclear spin zero. As a result they have no hyperfine structure. The alkali-metal atoms have, however, an extensive hyperfine structure, which complicates the theoretical description of cold collisions. The reason for this is that not only the number of states involved increases, but that also the collisional process is influenced through angular momentum decoupling and recoupling phenomena. This occurs because, the hyperfine splitting is of the same order of magnitude as the kinetic energy in cold collisions [22].

Unfortunately excited metastable rare gas atoms have a complicated fine structure. As a result very many diatomic potentials (40) are possible for the metastable rare gas atoms even if only the $\{(n - 1)\ell ns\}$ and $\{(n - 1)p^\ell np\}$ ($J = 5$) states are considered. The number of fine structure states involved is comparable to the number of hyperfine structure states involved for the alkali atoms. The important difference, however, is that the asymptotic energy differences between the diatomic states are in general much larger for the rare gases than for the alkali-metal atoms. The result is that for the rare gas atoms complications arise in the theoretical treatment of the potentials in the short-range instead of the long-range, which is sometimes the case for alkali-metal atoms [22].

Fortunately, we do not have this problem when we perform PAS in the MT on spin-polarized atoms. We then only have to consider the photo-associative transition from the initial doubly stretched (polarized) free ground state Ne* $|^3P_2, m_J = 2\rangle$ - Ne$^* |^3P_2, m_J = 2\rangle$ to the doubly stretched (polarized) molecular bound vibrational excited state Ne* $|^3P_2, m_J = 2\rangle$ - Ne** $|^3D_3, m_J = 3\rangle$, because in the double stretched (polarized) states no dipole-dipole couplings to other states are possible. Therefore, the main contribution to the excited state interaction potential is the resonant dipole interaction $C_3/r^3$.
in the asymptotic limit. Also the PA spectrum is not obscured by couplings to many other states.

Another advantage of only having spin-polarized atoms (or doubly stretched states) is, that they are forbidden to Penning (auto-) ionize (§ 1.5.1). As a result, heating due to ionization is strongly suppressed. Moreover, the line width of the PA-spectrum is much reduced.

4.4 Analytical expression of the PA-spectrum

4.4.1 The rate coefficient

As described in § 4.2, with PAS the loss of particles from the trap as a function of the laser frequency is measured. The loss of particles from the trap increases, when the laser frequency $\hbar \omega_L$ equals the energy difference between the 'ground' and bound excited states. This increase in the loss of particles from the trap thus depends on the probability for excitation to a bound excited state, characterized by a transition rate $\gamma_p$, and the decay rate of the bound state resonance, characterized by a decay rate $\gamma_D$ to a product state. The intensity of the PA-spectrum is now proportional to the total cross section for the inelastic process that forms product $p$ from the initial ground state times the velocity $v$ of the atom, averaged over the velocity distribution of the atom cloud. This process can be characterized by the rate coefficient $K_p(T, \omega_L)$ [26]:

$$K_p(T, \omega_L) = \left\langle \frac{\pi v}{k^2} |S_p(\varepsilon, \omega_L)|^2 \right\rangle.$$ (4.3)

Here $T$ is the temperature of the atoms, $\varepsilon = \hbar k^2/2\mu$ the asymptotic kinetic energy of the 'ground' state Ne*{(2p)5 3s} atoms with $k = 2\pi/\lambda$ their wave number, and $S_p(\varepsilon, \omega_L)$ the scattering matrix element for the process that forms product $p$ from the initial 'ground' state channel. The brackets $\langle \cdots \rangle$ imply an average over the distribution of initial velocities $v$.

If a Maxwell-Boltzmann distribution at temperature $T$ is assumed, the rate coefficient is given by [26, 37]:

$$K_p(T, \omega_L) = \frac{k_B T}{h Q_T} \int_0^\infty |S_p(\varepsilon, \omega_L)|^2 e^{-\varepsilon/k_B T} \frac{d\varepsilon}{k_B T},$$ (4.4)

where $Q_T = (2\pi \mu k_B T/h^2)^{3/2}$ is the translational partition function. At MT temperatures, the scattering term $S_p$ for an isolated resonance can be approximated by [26]:

$$|S_p(\varepsilon, \delta_v)|^2 = \frac{\gamma_p \gamma_e(\varepsilon)}{(\varepsilon - \hbar \delta_v)^2 + (\gamma/2)^2},$$ (4.5)

where $\hbar \delta_v(\omega_L) = E_v - \hbar \omega_L$ is the energy relative to the bound state. The total width of the bound excited state is $\gamma = \gamma_p + \gamma_e(\varepsilon) + \gamma_0$, where $\gamma_p/\hbar$ is the rate by which the bound state decays to the detected product $p$, $\gamma_e(\varepsilon)/\hbar$ the free-bound transition rate from the free ground state to the excited molecular bound state, and $\gamma_0/\hbar$ the decay rate due to other undetected processes.

For low light intensities Fermi's golden rule gives: $\gamma_e = 2\pi |\langle g, \varepsilon |V_{rad}(R)|e, v \rangle|^2$, which is directly proportional to the light intensity. Here, $|g, \varepsilon \rangle$ is the ground state continuum wave function, $|e, v \rangle$ the excited state discrete wave function, $V_{rad}(R) = -d(R) \cdot \vec{E}_L$ [38] the radiative coupling matrix element, with $\vec{E}_L$ the electric field of the laser light and $d(R)$ the molecular transition dipole moment. With low intensity is meant those intensities for which the free bound transition is not saturated. Or in

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other words, when the transition rate $\gamma / h$ of the free-bound transition is much smaller than the line width $\Gamma$ of the atomic $\text{Ne}^* \left| ^3P_2, m_J = 2 \right\rangle \leftrightarrow \text{Ne}^{**} \left| ^3D_3, m_J = 3 \right\rangle$ transition; i.e. $\gamma / h \ll \Gamma$. For these low intensities the total width of the bound excited state reduces to: $\gamma = \gamma_p + \gamma_0$.

In experiments, however, high laser intensities of the order of $4 \text{ W cm}^{-2}$ ($s_0 \approx 1000$), where $\gamma / h \sim \Gamma$, are generally used. This is necessary because the PA probe laser beam is only turned on for periods of typically $\sim 100 \mu s$. Only these high intensities yield a significant loss of atoms from the trap. Equation (4.5) becomes less accurate for these intensities.

4.4.2 Trap loss rate

The above described rate coefficient $K_p$ only yields a relative value of the photo-association spectrum. For experiments, the absolute value of the intensity of the spectrum is required. The loss of atoms from the trap due to the photo-association effect can be detected in several ways. First, ionization is an important loss process of PA of metastable neon. These ions can be detected using a channeltron. However, for the doubly stretched (polarized) metastable neon atoms, ionization is suppressed (§ 1.5.1). Second, the number of atoms remaining in the trap can be measured using fluorescence or absorption spectroscopy. Third all particles escaping from the trap, mostly metastable atoms, can be detected using a channeltron. Here, we concentrate on detecting the number of metastable atoms escaping from the trap, using a channeltron. The rate coefficient and the loss rate $N_{loss}$ are calculated as a function of both the laser detuning and the scattering length in § 4.6.

The loss rate is given by:

$$\dot{N}_{loss} = \int \int \int_{V_{\text{trap}}} K_p n^2 \left( \frac{\Omega}{4\pi} \right)_{\text{det}} DdV,$$

(4.6)

where $n$ is the density of atoms in the MT, $\left( \frac{\Omega}{4\pi} \right)_{\text{det}}$ the solid angle of the detector, $D$ the quantum efficiency of the detector and $V$ the volume of the MT.

Immediately after the transfer from MOT to MT, the temperature of the trapped atoms will increase, due to the transfer process. The volume and the density are then assumed to be equal to those in the MOT. The volume is equal to $V = 0.1 \text{ cm}^3$ and the density to $n = 10^{11} \text{ cm}^{-3}$. For simplicity, a uniform average density distribution is assumed. The average temperature is assumed to be $250 \mu K$, close to the Doppler limit (3.9), which is an upper limit to the temperature. The solid angle of our channeltron is equal to $\left( \frac{\Omega}{4\pi} \right)_{\text{chan}} = 5 \times 10^{-3} \text{ sr}$. The quantum efficiency of the channeltron for detecting metastable atoms is approximately $1$.

Substituting these characteristic values in equation (4.6), we find $\dot{N}_{loss} = 5.0 \times 10^{24} \text{ m}^{-3} \times K_p$, resulting in $\dot{N}_{loss} = 5.0 \times 10^8 \text{ s}^{-1}$ for a typical rate constant of $K_p = 10^{-10} \text{ cm}^3\text{s}^{-1}$ for $s_0 = 1000$. The atoms are irradiated for $\sim 100 \mu s$ with the PA probe beam, resulting in a loss of $5 \times 10^4$ atoms from the trap. Losses of this magnitude can easily be detected experimentally with a channeltron.

4.5 The free-bound transition rate

In this section the analytical expression for the transition rate $\gamma_{\ell}(\varepsilon, l) / h$ from the initial doubly stretched (polarized) free ground state $\text{Ne}^* \left| ^3P_2, m_J = 2 \right\rangle - \text{Ne}^{**} \left| ^3P_2, m_J = 2 \right\rangle$ to the doubly stretched (polarized) molecular bound vibrational excited state $\text{Ne}^* \left| ^3P_2, m_J = 2 \right\rangle - \text{Ne}^{**} \left| ^3D_3, m_J = 3 \right\rangle$ is given.
4.5.1 Ground and excited state wave function

Ground state

The collision of metastable Ne* with its twin can be treated as the scattering of a particle by a central potential \( V(\vec{r}) \) in a reduced mass picture \([10]\). The initial state of the system is a solution to the stationary Schrödinger equation \([14]\):

\[
\left[-\frac{\hbar^2}{2\mu} \nabla^2 + V(\vec{r})\right] \Psi(\vec{r}) = E\Psi(\vec{r}),
\]

(4.7)

where \( \mu = m_1m_2/(m_1 + m_2) \) is the reduced mass with \( m_1 = m_2 = m_{Ne*} \) the atomic mass of the metastable neon atoms, \( \Psi(\vec{r}) \) the wave function and \( E \) the energy of the eigenstates of the Schrödinger equation. Adopting spherical coordinates and separating variables yields solutions to the Schrödinger equation of the form:

\[
\Psi_{l,m}^n(r, \theta, \phi) = Y_{l,m}^n(\theta, \phi) y_l(r)/r,
\]

(4.8)

where \( Y_{l,m}^n(\theta, \phi) \) are the normalized angular wave functions, the so-called spherical harmonics, which are the eigenfunctions of \( \hat{l}^2 \) and directly proportional to the associated Legendre Polynomials \( P_l^m(\cos \theta) \). Furthermore, \( l \) is the orbital angular momentum quantum number, \( m \) its projection on the axis of quantization and \( y_l(r) \) is the solution to the radial Schrödinger equation \([14]\):

\[
\left[-\frac{\hbar^2}{2\mu} \frac{\partial^2}{\partial r^2} + V_{\text{centr}} + V(r) - E\right] y_l(r) = 0.
\]

(4.9)

Here \( V \) is the central potential and \( V_{\text{centr}} \) is the centrifugal potential, defined as:

\[
V_{\text{centr}} = \frac{l(l+1)\hbar^2}{2\mu r^2}.
\]

(4.10)

The general solution of the free ground states to the radial Schrödinger equation can be expanded into so-called partial waves \([2]\):

\[
\Psi(r, \theta) = \sum_{l=0}^{\infty} a_l(k) \frac{y_l(kr)}{r} P_l(\cos \theta),
\]

(4.11)

taking \( \vec{k} \) along the \( y \)-axis.

For free particles, or \( V = 0, |\Psi\rangle \) is a plane wave with radial behaviour \([2]\):

\[
y_{l,\text{free}}(kr) = A(k) k r j_l(kr),
\]

(4.12)

where \( j_l(kr) \) is the spherical Bessel function and \( k^2 = 2\mu E/\hbar^2 \). When \( kr \) increases from 0 to \( \infty \), \( y_{l,\text{free}}(kr) \) first increases as \( (kr)^{l+1} \) till it reaches the inflection point where \( kr = \sqrt{l(l+1)} \). After this point \( y_{l,\text{free}}(kr) \) oscillates between two extremes, which asymptotically approach, respectively, \(-A(k)\) and \(A(k)\). The asymptotic form of the radial wave function in a potential \( V \neq 0, y_l(r) \), and in zero potential, \( y_{l,\text{free}}(r) \), as \( r \to \infty \) equals, respectively \([2]\):

\[
y_l(\vec{r}) \to A(k) \sin (kr - \frac{\pi}{2} l + \eta_l)
y_{l,\text{free}}(\vec{r}) \to A(k) \sin (kr - \frac{\pi}{2} l),
\]

(4.13)
where $\eta_l$ is the asymptotic phase shift between the solution of the Schrödinger equation in zero and non zero potential. The asymptotic form of the stationary scattering wave solutions to Schrödinger's equation (4.9) in a potential $V \neq 0$ as $r \to \infty$ also satisfies [2]:

$$y_l(r) = e^{ikr\cos \theta} + f(\theta)\frac{e^{ikr}}{r}.$$  \hspace{1cm} (4.14)

Here

$$f(\theta) = \sum_{l=0}^{\infty} f_l P_l(\cos \theta),$$  \hspace{1cm} (4.15)

is the scattering amplitude, which can be expressed as a sum of Legendre polynomials $P_l(\cos \theta)$.

Expressing (4.14) as an expansion of Legendre Polynomials and combining equation (4.11), (4.13), (4.14) and (4.15), the coefficients $a_l$ and $f_l$ can be determined [10]:

$$f_l = \frac{(2l + 1)}{k} e^{im} \sin \eta_l,$$

$$a_l = (i)^l \frac{2l + 1}{k} e^{im}.$$  \hspace{1cm} (4.16)

The solution, $y_l(r)$, of the radial Schrödinger equation (4.9) can be obtained numerically, using Numerov's outward integration formula [6].

In the unbound ground state Ne* $\{(2p)^53s\} -$ Ne* $\{(2p)^53s\} (\varepsilon > U(\infty))$, the spectrum of eigenvalues is continuous, $\varepsilon = \hbar^2 k^2 / 2\mu > 0$. Therefore, the free ground state wave function cannot be normalized in the usual sense. In order to obtain reliable values of the transition rate $\gamma_l / \hbar$, the ground state wave function needs to be energy normalized:

$$\int_{0}^{\infty} \langle g, \varepsilon | g, \varepsilon' \rangle r^2 dr = \int_{0}^{\infty} \frac{y_{l,e}(r)}{kr} \frac{y_{l,e'}(r)}{kr} r^2 dr = \delta(\varepsilon - \varepsilon').$$  \hspace{1cm} (4.17)

Here $\delta(\varepsilon - \varepsilon')$ is the Dirac delta function of the energy. Substituting (4.13) into equation (4.17) yields the normalization amplitude of the ground state wave function:

$$A(k) = \sqrt{\frac{4\mu k}{2\pi \hbar^2}}.$$  \hspace{1cm} (4.18)

The energy normalized ground state wave function $|g, \varepsilon\rangle$ is now given in units of $(Jm^3)^{-1/2}$.

**Excited state**

The determination of the excited state wave function is in principle very similar to that of the ground state. Now, however, bound instead of free states are considered. A Ne* and Ne** atom form together a so-called 'diatomic molecule'. As a consequence two additional modes of motion should be taken into account. First, the molecule can rotate as a whole around the axis perpendicular to the internuclear axis, passing through the center of gravity and second, the atoms can vibrate relative to each other along the internuclear axis. The first motion is characterized by the total angular momentum $J$, the second process is characterized by the vibrational quantum number $v$. 

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Therefore, it is more appropriate to describe the bound excited states in a molecule-fixed frame instead of the usual lab-fixed frame. The correlation between these two frames is given in Appendix F. In the molecule-fixed frame the centrifugal potential of the excited state has the form [19]:

\[ V_{\text{centr}} = -\frac{\hbar^2}{2\mu r^2} [J(J + 1) - \Omega^2], \]  

(4.19)

where \( J \) is the total angular momentum. The rotational angular momentum \( \vec{l} \) of the diatomic molecule is always perpendicular to the internuclear axis. As a consequence, its projection on the internuclear axis \( m_l \) is always zero. On the other hand the projection \( \Omega \) of the total electronic angular momentum \( \vec{j} \) on the internuclear axis is equal to \( \Omega = 5 \), since we only consider doubly stretched states. As a result the total angular momentum \( \vec{J} = \vec{j} + \vec{l} \), is at least equal to \( J = 5 \) and its projection on the internuclear axis equals \( M = \pm 5 \).

For the excited bound molecular state the spectrum of eigenvalues is discrete, therefore the excited state wave function can be normalized in the usual way:

\[ \int_0^\infty \langle e, v | e, v \rangle r^2 dr = 1. \]  

(4.20)

The excited state wave function is then given in units of \((m)^{-3/2}\).

### 4.5.2 Analytical expression

In order to calculate the transition matrix element, both the ground and excited state wave functions and the atom-laser interaction should be represented in the same basis. The excited state wave function can be transformed into the lab-fixed frame using the Wigner functions [10, 19]. The ground \(|g, \epsilon\rangle\) and excited state \(|e, v\rangle\) wave functions are given by [10]:

\[ |g, \epsilon\rangle = |j_1 = 2, m_{j_1} = 2\rangle |j_2 = 2, m_{j_2} = 2\rangle \sum_{l=0}^\infty a_l(\epsilon) \frac{y_{l, \epsilon}(r)}{r} |l, m_l = 0\rangle, \]

\[ |e, v\rangle = \frac{\gamma_0 \Omega J(r)}{\sqrt{2}(-)^{J-\Omega}} \sum_{l} \langle J\Omega; j - \Omega|l0\rangle |j lJM\rangle \]

(4.21)

The transition rate is defined as:

\[ \gamma(t) = 2\pi \sum_{l=0}^\infty |\langle e, v | \vec{E} \cdot \vec{D} | g, \epsilon, l \rangle|^2 \]  

(4.22)

The transition matrix element in the lab-fixed frame is given by [10]:

\[ \langle e, v | \vec{E} \cdot \vec{D} | g, \epsilon, l \rangle = \sqrt{2\hbar \Omega_l a_l(\epsilon)} \left( \frac{2l + 1}{2J + 1} \right)^{1/2} \langle jm_j; lm_l | JM, J | jm - j; lm_l \rangle \]

\[ \times \int_0^\infty dr \ y_{\epsilon, J}(r) y_{l, \epsilon}(r), \]  

(4.23)
where

\[ \Omega_R = \frac{E_0 d}{\hbar \sqrt{2}} = \sqrt{\frac{I d}{\hbar^2 2E_0 c}}, \]

\[ d = \frac{e(\langle a_e J_e || L || a_g J_g \rangle / \sqrt{2J_e + 1}}, \]

\[ a_l = (i)^l \frac{2l + 1}{k} e^{-i\eta_l}. \]

Here \( \eta_l \) is the difference in phase between the ground state wave function in a zero and nonzero potential for \( r \to \infty \), \( \gamma, \epsilon, l \) the ground state wavefunction for partial wave \( k \), the wave number, \( d \) the reduced atomic dipole matrix element, \( \langle a_e J_e || d_L || a_g J_g \rangle \) the reduced matrix element of the transition (Appendix C), and \( E_0 \) the amplitude of the electric field of the laser light.

The first term in equation (4.23), \( \Omega_{R_1} \), is the Rabi frequency. The second term, \( a_l \) is an amplitude factor depending on \( \eta_l \) and \( k \) and thus the kinetic energy \( \epsilon \). The terms between brackets are the Clebsch Gordon coefficients of the transition between the doubly stretched states of \( \text{Ne}^* \) and \( \text{Ne}^{**} \) given by \( \langle jm_j; lm_l | J M_J \rangle \) (Appendix C). Here \( j \) is the total electronic angular momentum, \( l \) the rotational angular momentum and \( J \) the total angular momentum of the diatomic molecule. The parameters \( m_j, m_l \) and \( M_J \) are their respective projections on the quantization axis in the lab-fixed frame. Their values are respectively equal to: \( j = m_j = M_J = 5, m_l = 0, l = 0, 2, \ldots \) and \( J = 5 + l \). In our case the colliding atoms have identical quantum numbers and are bosons. In order to meet the resulting symmetry requirements only even partial waves contribute [16]. The last term, \( \int d r y^*_e y(r) y^g(r) \), is the Franck-Condon integral.

Since, for this transition, the rotational angular momentum \( \tilde{l} \) is conserved, ground state \( s \)-waves couple to excited state \( s \)-waves with \( J = j + l = 5 \), \( d \)-waves couple to \( J = 5, 6, 7 \) and \( g \)-waves couple to \( J = 5, 6, 7, 8, 9 \) excited states. Coherent contributions (interference of partial waves differing in \( l \)) cancel out in an atom trap [38], so only incoherent contributions need to be taken into account. This is not the case in an atomic beam. The transition rate in the lab-fixed frame (4.22) is now given in units of energy, since the dimension of \( [\tilde{E} \cdot \tilde{D}] \) is [J].

For ultra cold collisions the expressions for (defrate) and (overgangt) simplify, since only the \( l = 0 \) wave contributes significantly to the photo-association spectrum. This can be understood in the following way. A ground state atom with kinetic energy \( \epsilon \) approaches the Condon radius \( R_C \) from \( \infty \). If \( l > 0 \) and \( r > R_C \) the atom needs to cross a centrifugal potential barrier (4.10), before it will be able to reach a region of space where excitation to an upper bound level is probable. In ultra cold collisions, the height of the centrifugal barrier (4.10) is larger than the kinetic energy of the colliding atoms. Therefore, in ultra cold collisions, only the \( l = 0 \) wave contributes. As a result, we expect that the rotational structure will be negligible.

### 4.6 Numerical calculations

#### 4.6.1 Introduction

The loss rate (4.6) due to photo association in the MT is calculated with the Visual C++ program PAS2. The transition rate \( \gamma_l / \hbar \) from \( \text{Ne}^* \) \( \{^3P_2, m_J = 2\} \) - \( \text{Ne}^* \) \( \{^3P_2, m_J = 2\} \) to \( \text{Ne}^* \) \( \{^3P_2, m_J = 2\} \) - \( \text{Ne}^{**} \).
\[ |^3D_3, m_J = 3 \rangle \text{ is calculated using both this program and an adapted version of Doery's FORTRAN program nesp1new4. The Franck-Condon integral and the asymptotic phase shift of the ground state wave function in zero and nonzero potential } \eta \text{ are calculated with the latter program. After interpolation of the ground and excited state potentials, the ground and excited state wave functions are calculated using Numerov's integration formula [6].}

In the second program the loss rate due to photo-association is determined, using equations (4.3), (4.5), (4.6), (4.22), (4.23) and (4.24). The scattering length is determined, using equation (4.1) and (4.13).

In this section first the interpolated short- and long-range ground and excited state potentials are given in subsection 4.6.2. Next, the calculated ground an excited state wavefunctions are discussed in subsection 4.6.3. The asymptotic phase shift of the ground state wavefunction and the scattering length as a function of the phase integral, which characterizes the different ground state potentials, are calculated in subsection 4.6.4, for \(^{20}\text{Ne}^*\) as well as \(^{22}\text{Ne}^*\). Then, the PA spectra for a couple of different ground state potentials are presented in subsection 4.6.5. Also the rotational structure is calculated for one potential and one bound excited vibrational level.

Unless indicated otherwise, the wavefunction, potential, phase shift, scattering length or loss rate of \(^{20}\text{Ne}^*\) is considered.

### 4.6.2 Interaction potentials

As input potentials are used the short range \(\text{Ne}_2 A_g\) and \(\text{Ne}_2 5u\) potentials of Kotochigova et al. [28], for the ground and excited state, respectively. These short range potentials are used to interpolate the total potential including long-range effects.

The long-range ground \(U_g\) and excited state \(U_e\) potentials are given by:

\[
\begin{align*}
U_g(r) &= C_6 \frac{1}{r^6} + \frac{l(l+1)\hbar^2}{2\mu r^2} \\
U_e(r) &= C_3 \frac{1}{r^3} + \frac{[J(J+1) - 25]h^2}{2\mu r^2} + i\Gamma.
\end{align*}
\]

Here \(\frac{C_6}{r^6}\) is the long-range induced dipole interaction of the ground state potential. The resonant dipole interaction of the excited molecular potential is described by \(\frac{C_3}{r^3}\) and \(i\Gamma\) takes the decay of the excited state into account.

Figure 4.2 shows the short-range potentials as a function of \(r\). The ground state potential is minimum at \(r_{\text{min}} = 9.95 \, \text{a}_0\) and the well depth at \(r_{\text{min}}\) is equal to \(U_{\text{min}} = -315.5\, \text{K}\). The centrifugal barriers of the ground state potential for \(l = 2\) and \(l = 4\) are located at \(r \approx 78\, \text{a}_0\) and \(r \approx 58\, \text{a}_0\), respectively, and are equal to \(U_g = 16\, \text{mK}\) and \(35\, \text{mK}\), respectively. So, our atoms with kinetic energies of the order of \(100\, \mu\text{K}\) will not be able to cross these centrifugal barriers.

The excited state potential is minimum at \(r_{\text{min}} = 6.23\, \text{a}_0\) and the well depth at \(r_{\text{min}}\) is equal to \(U_{\text{min}} = -12658.6\, \text{K}\). For the excited state potential, (Figure 4.2b), also the highest calculated vibrational level \(v = 147\) is given. The vibration energy of this bound state is \(E_{147} = -0.12528\, \text{K}\) relative to the dissociation limit, and has turning points at \(r = 3.99\, \text{a}_0\) and \(r = 255\, \text{a}_0\).

The \(C_3\) and \(C_6\) coefficients are obtained by diagonalization of a Hamiltonian matrix containing the atomic energies and the electric dipole-dipole interaction, deduced from experimentally determined
4.6 Ground and excited state wave functions

Figure 4.3 shows the ground state wavefunction as a function of the interatomic distance, for two different ground state interaction potentials of $^{20}\text{Ne}^*$. The wavefunction curving upwards (solid line) has a negative scattering length $a = -42 \text{ a}_0$ and is characterized by a phase integral $\phi = 16.33 \pi$. The phase integral gives the number of bound states the potential can support. A phase integral of $\phi = 16.33 \pi$ means that the potential supports 16 bound states.

The long-range part of the wavefunction is fitted with $\sin(k(r-a))$ (4.13) (dashed line). This fit gives a clear picture of the scattering length: the scattering length is the effective point of origin of the long-range wave function. The long-range wave function intersects with the $x$–axis at $r = a = -42 \text{ a}_0$. The period of the long-range wave function is for $T = 250 \mu\text{K}$ equal to 1170 $\text{a}_0$, corresponding to $\approx 0.1\lambda$, with $\lambda$ the wavelength of the transition.

The wavefunction curving downwards (solid line) has a positive scattering length $a = +42 \text{ a}_0$ and is characterized by a phase integral $\phi = 17.10 \pi$. The fit of the long-range wavefunction (dotted line) is, however, better for a scattering length of $a = +32 \text{ a}_0$.

In the range $3 - 25 \text{ a}_0$ in the well region of the ground state potential (Figure 4.2 a), the wavefunctions oscillate rapidly, due to an increase in the kinetic energy at smaller internuclear separations. Also because of the high velocity of the atoms, the amplitude of the wavefunction in this region and...
Figure 4.3: Ground state wavefunctions as a function of the interatomic separation. Two ground state wavefunctions for two different ground state interaction potentials are shown. The wavefunction curving upwards (solid line) has a negative scattering length $a = -42 \, a_0$ and is characterized by a phase integral $\phi = 16.33 \, \pi$. The wavefunction curving downwards (solid line) has a positive scattering length $a = +42 \, a_0$ and is characterized by a phase integral $\phi = 17.10 \, \pi$. For both wavefunctions the fit of the long-range wavefunction is shown (dashed and dotted line, respectively).
Figure 4.4: Two bound excited state wavefunctions as a function of the interatomic separation. The solid line shows the $v = 147$ bound vibrational state, where $v$ is vibrational quantum number and $v = 0$ corresponds to the lowest bound vibrational state in the potential well. The dashed line corresponds to the wave function of the $v = 146$ bound vibrational level. The curves clearly show that the probability amplitude is maximum near the outer turning points of the vibrational bound states.

thus the probability that the atoms will get so close together is very small. In addition, the cross section $\sigma = \pi r^2$ for scattering is much smaller at small interatomic distances.

Figure 4.4 shows two bound excited state wavefunctions as a function of the interatomic separation. The two curves correspond to the $v = 147$ (solid line) and $v = 146$ (dashed line) bound vibrational level, respectively. Here $v$ is the vibrational quantum number and $v = 0$ corresponds to the lowest vibrational bound state in the potential well. The vibrational energies of these states are, respectively, $E_{147} = -0.1253$ K and $E_{146} = -0.1639$ K with respect to the dissociation energy. The outer turning points for these excited vibrational states are, respectively, equal to $r_{147} = 255 a_0$ and $r_{146} = 233 a_0$. Their inner turning points are the same and equal to $r_{inner} = 3.99 a_0$.

From Figure 4.4 it is clear, that the amplitude of these excited state wavefunctions is maximum near the outer turning point, as expected. For smaller interatomic separations the amplitude of the wavefunction and thus the probability amplitude is much smaller and steadily decreases. At the inner turning point a small local maximum occurs, since almost all kinetic energy of the atoms has been transferred into potential energy at this point and consequently the atoms spend here more time. Also the wavefunction starts to oscillate more rapidly for smaller interatomic separations, due to an increase in the kinetic energy at smaller interatomic separations.
Figure 4.5: The phase of the ground state potential for three different partial waves $l = 0, 2, 4$ as a function of the interatomic distance $r$. The phase relations shown are calculated for an atom with kinetic energy $\varepsilon = 200 \mu K$ and ground state interaction potential with phase integral $\phi_0 = 17.20 \pi$. The asymptotic phase is linear in $r$. The phase shift between the different partial waves is $\Delta \phi \approx \pi$.

4.6.4 Phase shift and scattering length

The asymptotic phase difference between the ground state wave function in zero and nonzero potential has been determined by fitting the asymptotic phase of the ground state wave function as a function of $r$. Figure 4.5 shows the phase of the long-range ground state wave function as a function of the interatomic distance between the atoms, for atoms with a ground state kinetic energy $\varepsilon = 200 \mu K$ in an unchanged ground state potential with $\phi_0 = 17.20 \pi$ and for $l = 0, 2, 4$. In the asymptotic limit the ground state wave function is a sine (4.13). Therefore, the asymptotic phase is linear in $r$ for large $r$. The slope of the fit of the asymptotic phase is equal to the wave number $k = \frac{\sqrt{2m\varepsilon}}{\hbar}$ and the intercept with the $y$-axis gives the asymptotic phase shift $\eta_l$. The picture clearly shows that the phase shift between the different partial waves is of the order $\pi$, in agreement with theory (4.13). The scattering length is now calculated from $\eta_0$ using equation (4.1). The uncertainty in $a$, due to fitting the asymptotic phase shift of the ground state wave function, is much smaller than $1 a_0$.

It is not precisely clear how accurate this method to determine $a$ is. Of course, the real value of the scattering length can only be determined from comparing experiments with calculations. The asymptotic phase shift and thus the scattering length are calculated at $T = 200 \mu K$, since, at temperatures around $50 \mu K$, the reliability of the calculations of the wave functions is questionable. Because equation (4.1) only holds in the low temperature limit, the scattering lengths calculated here are only an approximation.
The ground state molecular potential is now varied by adding a Gaussian bump to the potential well in such a way that its phase integral can be changed over an interval \([0, \pi]\). For each of these potentials the loss of atoms from the MT, due to photo-association from the doubly stretched \(^3\text{P}_2, m_J = 2\) - \(^3\text{P}_2, m_J = 2\) to the \(^3\text{P}_2, m + J = 2\) - \(^3\text{D}_3, m_J = 3\) states, and the scattering length are calculated.

Figure 4.6 shows the scattering length of metastable \(^{20}\text{Ne}^*\) and its isotope \(^{22}\text{Ne}^*\), as a function of the phase integral \(\phi\) of the ground state interaction potential. A ground state potential changed by a certain amount has a phase integral \(\phi_{20}\) for \(^{20}\text{Ne}^*\) and a phase integral \(\phi_{22}\) for \(^{22}\text{Ne}^*\). The phase integral \(\phi_{22}\) of \(^{22}\text{Ne}^*\) is related to the phase integral \(\phi_{20}\) of \(^{20}\text{Ne}^*\) as:

\[
\phi_{22} = \sqrt{\frac{m_{22}\text{Ne}^*}{m_{20}\text{Ne}^*}} \phi_{20}.
\]  

The scattering length of both isotopes is plotted for potentials changed by the same amount. The lower and upper \(x\)-axes give, respectively, the corresponding phase shift of \(^{20}\text{Ne}^*\) and \(^{22}\text{Ne}^*\).

Both curves display clearly a singularity in the scattering length at \(\phi_{20} \approx 16.25\ \pi\) and \(16.65\ \pi\), respectively. These resonances in the scattering length and thus the elastic collision cross section \(\sigma_{el}\) occur due to a 'zero-energy' resonance, the potential is nearly too weak to support the highest bound state (virtual state).

The scattering length changes from positive to negative at \(\phi_{20} \approx 16.25\ \pi\) and \(16.39\ \pi\) for \(^{20}\text{Ne}^*\) and \(^{22}\text{Ne}^*\), respectively. Thus is 15% of the total phase interval \([0, \pi]\) is the scattering length of \(^{20}\text{Ne}^*\) negative but the scattering length of \(^{22}\text{Ne}^*\) positive.

The scattering length is only negative for both isotopes for potentials characterized by a phase integral between \(16.39 < \phi_{20} < 16.50\ \pi\). So, only for 10% of the total phase interval \([0, \pi]\) is the scattering length of \(^{20}\text{Ne}^*\) as well as \(^{22}\text{Ne}^*\) negative. Thus when the scattering length of \(^{20}\text{Ne}^*\) proves to be negative, there is a large possibility that the scattering length of its isotope \(^{22}\text{Ne}^*\) is positive.

4.6.5 Loss rate due to PAS

In order to obtain doubly stretched states the atoms are transferred from the MOT to the MT and spin polarized. The temperature, density and the size of the MT, immediately after the transfer from the MOT, are \(T = 250\ \mu\text{K}\), \(n = 10^{11}\ \text{cm}^{-3}\) and \(V = 0.1\ \text{cm}^3\). The photo association is induced with a right hand circularly polarized \((\sigma^+)^\text{PA}\) probe laser beam, which is applied for typically \(\sim 100\ \mu\text{s}\).

In the calculations \(\gamma_p\) is chosen equal to the spontaneous emission rate \(\gamma_s = 3.4 \times 10^{-26}\ \text{J}\), which yields a lower limit to \(\gamma_p\). Furthermore, \(\gamma_0 = 0\) is assumed. A saturation parameter of \(s_0 = 1000\) [35] for the intensity of the scanning PA laser beam, has been used to obtain the loss rate. The rate constant \(K_p\) for loss due to photo-association is calculated for a saturation parameter \(s_0 = 1\). From this rate constant \(K_p\) the loss rate can easily be calculated for different experimental conditions and detection methods, using equation (4.6).

Photo-association spectra

Figure 4.7 shows the photo-association spectrum as a function of the probe laser detuning from the dissociation limit, for Kotochigova's unchanged ground state interaction potential [28], characterized by a phase integral \(\phi = 17.20\ \pi\) and a scattering length \(a = +29\ a_0\). The loss rate (and the rate
Figure 4.6: The scattering length of metastable $^{20}\text{Ne}^*$ and its isotope $^{22}\text{Ne}^*$, as a function of the phase integral of the ground state interaction potential. The lower and upper $x-$axis show, respectively, the phase integral of the ground state potential of $^{20}\text{Ne}^*$ and $^{22}\text{Ne}^*$, corresponding to the same change in the potential. Clearly, an interval exists where the scattering length of $^{20}\text{Ne}^*$ is negative but the scattering length of $^{22}\text{Ne}^*$ is positive.

Figure 4.7: The photo-association spectrum as a function of the probe laser detuning from the dissociation limit, for the unchanged ground state interaction potential, characterized by a phase integral $\phi = 17.20\,\pi$ and a scattering length $a = +29\,a_0$. The loss rate of atoms from the trap due to photoassociation shows a peak, whenever the probe laser frequency is tuned to a vibrational excited bound state resonance.
constant) of atoms from the trap due to photo-association $N_{\text{loss}}$ shows a peak, whenever the PA probe laser frequency is tuned to a vibrational excited bound state resonance. The loss rate changes from $7 \times 10^8$ to $2 \times 10^8$ atoms/s for $s_0 = 1000$ and the rate constant changes from $14 \times 10^{-14}$ to $4 \times 10^{-14}$ cm$^3$s$^{-1}$ for $s_0 = 1$ at resonance. Figure 4.8 also shows a photo-association spectrum as a function of the probe laser detuning from resonance, only for a ground state potential characterized by a phase integral $\phi = 16.53 \pi$ and a scattering length $a = +260 \ a_0$. The line width of the peaks are approximately $1.5 \ \Gamma$ for all PA spectra, and are due to spontaneous decay of the excited state and power broadening. The rotational structure is not taken into account, which is a good approximation as we will see below.

Both figures clearly show that the loss rate $N_{\text{loss}}$ varies for different excited vibrational bound levels, due to Frank-Condon oscillations. This is especially clear for the spectrum shown in Figure 4.8; the loss rate and the rate constant decrease dramatically when the laser is tuned to the $v = 143$ bound vibrational level. The loss rate decreases from $4.4 \times 10^8$ for $v = 147$ to $0.11 \times 10^8$ atoms/s for $v = 143$, and the rate constant from $9 \times 10^{-14}$ to $0.22 \times 10^{-14}$ cm$^3$s$^{-1}$. Since only the overlap integral at the range of $r$ closely surrounding the outer turning point of the excited vibrational level contributes to the transition rate $\gamma_i/\hbar$, the transition rate is proportional to the amplitude of the ground state wavefunction. Apparently, the ground state wavefunction has a node at the outer turning point of the $v = 143$ bound vibrational level. The outer turning point for this vibrational level is equal to $r_{143} = 182 \ a_0$. And indeed, this ground state wavefunction has a node at $r = 183 \ a_0$. The outer turning points and the vibrational energies of a number of the highest excited bound vibrational levels are given in Table 4.1. The position of the nodes of the ground state wavefunction are directly related

Figure 4.8: The photo-association spectrum as a function of the probe laser detuning from the dissociation limit, for a ground state interaction potential, characterized by a phase integral $\phi = 16.53 \pi$ and a scattering length $a = +260 \ a_0$. The loss rate of atoms from the trap due to photo-association shows a peak, whenever the probe laser frequency is tuned to a vibrational excited bound state resonance.

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Figure 4.9: The loss rate and rate constant at excited bound vibrational resonances for five different ground state potentials. The loss rate and rate constant are plotted as a function of the outer turning points of the highest excited bound vibrational levels. These curves are the intensity envelopes of the photo-association spectrum and display clearly Frank-Condon oscillations.

to the scattering length of the ground state potential.

Figure 4.9 show the loss rate and rate constant at excited bound vibrational resonances for five different ground state potentials. The loss rate and rate constant are plotted as a function of the outer turning points of the highest excited bound vibrational levels. The phase integral and the scattering length of these five potentials are given in Table 4.2. These curves are the intensity envelopes of the photo-association spectrum and clearly display Frank-Condon oscillations. The loss rate is on average of the order $10^8$ atoms/s, and the rate constant is of the order $10^{-14} - 10^{-13}$ cm$^3$s$^{-1}$ at photo-associative resonances for $s_0 = 1$.

The photo-association spectrum of the curve characterized by $\phi_1 = 16.53 \pi$ was already discussed above. The envelope of the photo-association spectrum, characterized by $\phi_2 = 16.49 \pi$ has a minimum near $r = 233 a_0 (v = 146)$. This is close to the node, $r = 249 a_0$, of the ground state wavefunction belonging to this potential, which lies between the outer turning point of the $v = 147$ and $v = 146$ vibrational levels.

The remaining curves, characterized by $\phi_0, \phi_3$ and $\phi_4$, display no minima, because the first node of their long-range ground state wavefunctions all lie between 550 and 600 $a_0$ (Table 4.9). This means that their long-range ground state wavefunctions have a maximum in the range 260 to 310 $a_0$. And indeed, the envelopes of their PA spectra seem to have a very wide maximum in this range.

So the behaviour of the ground state wavefunction is directly reflected in the envelope of the photo-association spectrum. The position of the nodes of the ground state wavefunction can be determined from these envelopes. These nodes are related to the scattering length of the potential. On the other hand, Figure 4.9 also shows that the envelopes are clearly no simple sines squared. This
Table 4.1: Vibrational energies and outer turning points $r_{outer}$ for the highest bound vibrational levels of the excited state interaction potential.

<table>
<thead>
<tr>
<th>$v$</th>
<th>$E_v$ (K)</th>
<th>$r_{outer}$ (a₀)</th>
</tr>
</thead>
<tbody>
<tr>
<td>147</td>
<td>-0.1253</td>
<td>255</td>
</tr>
<tr>
<td>146</td>
<td>-0.1639</td>
<td>233</td>
</tr>
<tr>
<td>145</td>
<td>-0.2119</td>
<td>214</td>
</tr>
<tr>
<td>144</td>
<td>-0.2711</td>
<td>197</td>
</tr>
<tr>
<td>143</td>
<td>-0.3435</td>
<td>182</td>
</tr>
<tr>
<td>142</td>
<td>-0.4307</td>
<td>169</td>
</tr>
<tr>
<td>141</td>
<td>-0.5356</td>
<td>157</td>
</tr>
<tr>
<td>140</td>
<td>-0.6598</td>
<td>147</td>
</tr>
<tr>
<td>139</td>
<td>-0.8081</td>
<td>137</td>
</tr>
<tr>
<td>138</td>
<td>-0.9837</td>
<td>128</td>
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<tr>
<td>137</td>
<td>-1.1882</td>
<td>121</td>
</tr>
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<td>136</td>
<td>-1.4294</td>
<td>113</td>
</tr>
<tr>
<td>135</td>
<td>-1.7015</td>
<td>107</td>
</tr>
<tr>
<td>134</td>
<td>-2.0367</td>
<td>101</td>
</tr>
<tr>
<td>133</td>
<td>-2.4030</td>
<td>95</td>
</tr>
<tr>
<td>132</td>
<td>-2.8388</td>
<td>90</td>
</tr>
<tr>
<td>131</td>
<td>-3.3341</td>
<td>86</td>
</tr>
<tr>
<td>130</td>
<td>-3.8878</td>
<td>81</td>
</tr>
<tr>
<td>129</td>
<td>-4.5441</td>
<td>77</td>
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<tr>
<td>128</td>
<td>-5.2660</td>
<td>73</td>
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<tr>
<td>127</td>
<td>-6.0924</td>
<td>70</td>
</tr>
<tr>
<td>126</td>
<td>-7.0329</td>
<td>67</td>
</tr>
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<td>125</td>
<td>-8.0842</td>
<td>64</td>
</tr>
<tr>
<td>124</td>
<td>-9.2483</td>
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<td>123</td>
<td>-10.5711</td>
<td>58</td>
</tr>
<tr>
<td>122</td>
<td>-12.0476</td>
<td>56</td>
</tr>
<tr>
<td>121</td>
<td>-13.6789</td>
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</tr>
<tr>
<td>120</td>
<td>-15.4959</td>
<td>51</td>
</tr>
</tbody>
</table>
Table 4.2: Phase integral, scattering length and relevant nodes of the ground state wavefunction for five different ground state interaction potentials. The loss rate and rate constant for these five potentials are given in Figure 4.9.

<table>
<thead>
<tr>
<th>$\phi$ ($\pi$)</th>
<th>$a$ ($a_0$)</th>
<th>node ($a_0$)</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\phi_0$</td>
<td>17.20</td>
<td>+29</td>
</tr>
<tr>
<td>$\phi_1$</td>
<td>16.53</td>
<td>+260</td>
</tr>
<tr>
<td>$\phi_2$</td>
<td>16.49</td>
<td>-393</td>
</tr>
<tr>
<td>$\phi_3$</td>
<td>16.33</td>
<td>-42</td>
</tr>
<tr>
<td>$\phi_4$</td>
<td>16.24</td>
<td>+1.7</td>
</tr>
</tbody>
</table>

is what we might expect, since the long-range ground state wavefunction is a sine and the overlap integral is proportional to the ground state wavefunction. The rate constant and loss rate are directly proportional to the transition rate $\gamma / \hbar$ (at low intensities), which is in its turn directly proportional to the overlap integral squared. A more complicated expression for the overlap integral is necessary to fit the envelopes, since, although, the main contribution to the overlap integral is the overlap between the ground and excited state wavefunction at the outer turning point of the bound excited vibrational state, also larger $r$ contribute to the overlap integral (Figure 4.4). Taking into account the shape of the excited state wavefunctions may yield a good fit of the envelopes. From these fits, the scattering length could then be determined.

Rotational structure

Figure 4.10 shows the rotational structure of the $v = 147$ bound vibrational state. Partial waves with $l = 0, 2$ and 4 couple, respectively, to excited states with $J = 5$, $J = 5, 6, 7$ and $J = 5, 6, 7, 8, 9$. From Figure 4.10 a and b, it is clear that only the $J = 5$ excited state contributes significantly to the photo-association spectrum. For each increase in $J$ with one, the loss rate decreases by more than an order of magnitude. These pictures also show that the ro-vibrational energy $E_{v,J}$ increases for increasing $J$ (the resonance peak moves to the right). The ro-vibrational energies for the $v = 147$ vibrational excited bound state are given in Table 4.3.

The rotational structure might contribute significantly to the photo-association spectrum when quasibound resonances occur. These resonances can occur when the asymptotic phase shift and therefore the cross section for excitation varies rapidly in a certain energy range. These resonance are only possible for partial waves with $l \neq 0$. Such a resonance might occur, for example, when the ground state energy is equal to the vibrational energy of a quasi-bound state, supported by the centrifugal barrier of the ground state potential. When this is the case and the bound states lie at high energies (just barely bound states), there is a finite probability for the ground state atoms to tunnel through the centrifugal barrier and form a relatively long lived metastable state. The atoms will under go a number of vibrations before they exit and spend therefore a relatively large amount of time in this region. As a result the probability for excitation might increase and thus also the loss rate due to photo-association.
a) Rotational structure for $J = 5, 6$

b) Rotational structure for $J = 7, 8$

Figure 4.10: The rotational structure for the $v = 147$ vibrational bound state and Kotochigova's [28] unchanged ground state potential. The loss rate as a function of the detuning from resonance is shown for, a, $J = 5, 6$ and, b, $J = 7, 8$. It is clear that only $J = 5$ contributes significantly to the photo-association spectrum.

Table 4.3: Ro-vibrational energies for the $v = 147$ vibrational excited bound state of Kotochigova's [28] unchanged ground state potential.

<table>
<thead>
<tr>
<th>$J$</th>
<th>$E_{v,J}$ (K)</th>
</tr>
</thead>
<tbody>
<tr>
<td>5</td>
<td>-0.1253</td>
</tr>
<tr>
<td>6</td>
<td>-0.1207</td>
</tr>
<tr>
<td>7</td>
<td>-0.1155</td>
</tr>
<tr>
<td>8</td>
<td>-0.1096</td>
</tr>
<tr>
<td>9(^a)</td>
<td>-0.1375</td>
</tr>
</tbody>
</table>

\(^a\)Belonging to the $v = 146$
vibrational excited bound state.
4.7 Conclusions

Only in a small interval, \( \approx 10\% \) of the total phase uncertainty interval \([0, \pi]\), the scattering length is negative for both \(^{20}\text{Ne}^*\) and \(^{22}\text{Ne}^*\). So the prospects are promising that the scattering length is positive and that BEC is possible for at least one of the two metastable neon isotopes.

The photo-associative loss rate is on average of the order \(10^8\) atoms/s, and the rate constant is of the order \(10^{-14} - 10^{-13} \text{ cm}^3\text{s}^{-1}\) at photo-associative resonances for \(s_0 = 1\). Comparing these photo-associative rate constants with the predicted rate constant for \(s-s\) ionization in a spin polarized gas \(\kappa_{\text{ion}}^{\text{pol}} \leq 5 \times 10^{-15} \text{ cm}^3\text{s}^{-1}\) (1.7), we can conclude that it is no problem to measure the photo-associative loss rate. In an unpolarized gas, however, the photo-associative rate constant \(K_p\) is less or at best equal to the rate constant for ionization \(\kappa_{\text{ion}}\). When light assisted ionization occurs, the situation is even worse.

At the pressures currently available in our trapping chamber, the loss rate due to collisions with the background gas is also much smaller than the loss rate due to photo-association, since this loss rate goes with the density of the background gas \(n_{\text{gas}} \approx 3 \times 10^7 \text{ cm}^{-3}\) at \(T = 300\text{K}\), resulting in a loss rate of \(\dot{N}_{\text{loss}} = 2.4 \times 10^6\) atoms/s. Thus PAS is well feasible.

The behaviour of the ground state wavefunction is directly reflected in the envelope of its photo-association spectrum. The position of the nodes of the ground state wavefunction can be determined from these envelopes. However, these envelopes cannot be fit with a simple expression, in order to determine directly the scattering length from experimental PA spectra. A more complicated expression for the overlap integral is necessary to fit the spectra and is one of the future goals.

In general, the contribution of the rotational structure to the PA spectrum is negligible.

The quantitative uncertainty of the calculations is not known. The calculated spectra give, however, information about the order of magnitude of the loss rate and photo-associative rate constant to be expected experimentally. A first step is made towards determining the scattering length from PA experiments.
Prospects are favorable that in the near future Bose-Einstein condensation (BEC) of metastable neon will be realized at Eindhoven University of Technology. The magnetic trapping fields of both the MOT and the MT meet, after adapting the design of Stas [34], the trapping requirements necessary to achieve BEC. The trapping requirements are a weak confinement during the transfer from MOT to MT, to minimize loss in phase space density during the transfer and to transfer as many atoms as possible, a tight confinement during the evaporative cooling phase, and a minimum magnetic field strength which is positive and of the order of 1 G. All these requirements have been verified experimentally. Everything is ready to start loading and optimizing the MT.

The MOT is operational and, although it needs further optimization, already at least $5 \times 10^8$ trapped atoms have been observed. At least, since recent absorption imaging experiments seem to indicate that the number of trapped particles in the MOT is underestimated in the fluorescence spectroscopy measurements. An explanation for this can be found in the fact that the reradiated light by the trapped atoms, the fluorescence, is always resonant. Therefore, the cross section for absorption of reradiated light is larger than the cross section for absorption of the laser light, for non zero laser detunings. As a result, part of the reradiated light is absorbed by the atoms, and consequently the number of particles measured with fluorescence spectroscopy is underestimated. Systematic absorption measurements should give in the near future a decisive answer about the absolute number of particles in the MOT.

At the densities $\sim 10^{10}$ cm$^{-3}$ and background pressure $\sim 10^{-9}$ mbar in our MOT, loss of atoms from the trap due to ionization is the dominant loss process. The measured ionization rate constant is for low and high magnetic field gradients of the order of $\beta_{\text{ion}} \approx 10^{-9}$ cm$^3$s$^{-1}$. This value is larger than the ionization rate constant $\kappa_{\text{ion}} = 5 \times 10^{-11}$ calculated by Doery et al (1.7) [23] because light assisted collisions between Ne* (3s) and Ne** (3p) atoms occur in our MOT. Our measurements on the light assisted ionization rate constant are consistent with comparable measurements on triplet metastable helium [25]. In the near future, measurements on the decay of the MOT in the absence of light assisted collisions will be performed, to determine the the ionization rate due to $s-s$ collisions, experimentally. Also, after the MT has been made operational, the rate constant for ionization of polarized atoms in the MT will be measured.

The observed lifetime of the MOT $\sim 30$ ms is long enough to cool the atoms in the MOT to the sub-Doppler limit ($\tau \sim 1$ ms) and to successively transfer them from the MOT to the MT ($\tau_{\text{transfer}} \sim 1$ ms). The MOT needs, however, to be optimized further to obtain the desired number of trapped particles.
Concluding remarks

particles, $10^{10}$ atoms, and MOT volume 0.1 cm$^3$ (in recent experiments $1 \times 10^{10}$ trapped atoms have been observed in a MOT volume of $\sim 1.5$ cm$^3$).

Calculations on photo-association spectroscopy (PAS) indicate a very large probability that at least one of the two isotopes of neon has a positive scattering length and that thus BEC of at least one of the two isotopes is feasible. Because the interaction potential of metastable neon is not known, the calculations are carried out for slightly different ground state potentials, characterized by a phase integral. Only in a small interval, $\approx 10\%$ of the total phase uncertainty interval $[0, \pi]$ over which the phase integral is varied, is the scattering length negative for both $^{20}\text{Ne}^*$ and $^{22}\text{Ne}^*$.

The photo-associative loss rate is on average of the order $10^8$ atoms/s, and the rate constant is of the order $10^{-14} - 10^{-13}$ cm$^3$s$^{-1}$ at photo-associative resonances for $s_0 = 1$. In general, the contribution of the rotational structure to the PA spectrum is negligible.

Comparing these photo-associative rate constants with the predicted rate constant for $s - s$ ionization in a spin polarized gas $K_{\text{ion}}^{\text{pol}} \leq 5 \times 10^{-15}$ cm$^3$s$^{-1}$ (1.7), we can conclude that it is no problem to measure the photo-associative loss rate. In an unpolarized gas, however, the photo-associative rate constant $K_p$ is less or at best equal to the rate constant for ionization $K_{\text{ion}}$. Therefore, future photo-association measurements should be performed in the MT, after spin-polarizing the atoms. The loss rate due to photo-ionization is also much larger than the loss rate due to collisions with the background gas. Thus PAS is well feasible.

Although the behaviour of the ground state wavefunction and thus the scattering length is reflected in the calculated PA spectra, it is not yet possible to obtain the scattering length from a fit of a measured PA spectrum. One of our goals in the near future is to be able to fit experimental PA spectra, to determine immediately the scattering length of metastable neon from the measurements.

The quantitative uncertainty of the calculations is not known. The calculated scattering lengths are only an approximation, since they have been calculated at finite temperatures and the interaction potential of metastable neon is not known. An improvement in the accuracy of the calculations, by calculating the temperature averaged photo-associative rate constant for the complete range of temperatures in the MT, is desirable and will be performed in the near future. However, because of the many unknown (or not accurately known) parameters in our calculations (the ground and excited state interaction potentials, $\gamma_p$, the natural decay time, etc.), it is more worthwhile to first compare the calculations to PA measurements on metastable neon.
Bibliography


[21] Homepage MIT.


Appendix A

Analytical description of the magnetic fields

A.1 The magnetic fields of the MT

Figure A.1 shows the simplified coil configuration, which Stas [34] used to illustrate the magnetic fields of the Clover Leaf trap. In order to derive a simple analytical expression for the magnetic trapping field each turn is approximated by a closed loop of thin wire. The Bias and Pinch coils are approximated by single loops of radius $R$, a distance $2A$ apart.

Figure A.2 shows how the Gradient coils are approximated in the calculations. The eight Gradient coils, schematically depicted in Figure A.2 a), are each approximated by two straight and two elliptic wire segments (Figure A.2 b). It turns out that the contributions from the two elliptical parts cancel each other [34]. Consequently, each of the Gradient coils can be approximated by a pair of straight wire segments as depicted in Figure A.1 and A.2 c).

The magnetic field from a single circular loop of radius $R$, perpendicular to the $z-$axis and centered at $z = A$ which carries a steady current $I$ has, due to symmetry, an azimuthal magnetic field component $B_\phi = 0$ and axial and transverse components [33]:

$$
B_r = \frac{\mu_0 I}{2\pi r} \frac{z - A}{((R + r)^2 + (z - A)^2)^{1/2}} \left( -K(k^2) + \frac{R^2 + r^2 + (z - A)^2}{(R - r)^2 + (z - A)^2} E(k^2) \right),
$$

$$
B_z = \frac{\mu_0 I}{2\pi r} \frac{1}{((R + r)^2 + (z - A)^2)^{1/2}} \left( K(k^2) + \frac{R^2 - r^2 - (z - A)^2}{(R - r)^2 + (z - A)^2} E(k^2) \right).
$$

(A.1)

Where $K$ and $E$ are respectively the complete elliptic integral of the first and second kind and $\mu_0$ is the magnetic permeability of vacuum and $k^2$ is given by:

$$
k^2 = \frac{4Rr}{(R + r)^2 + (z - A)^2}.
$$

(A.2)

On the $z-$axis we find $B_r \to 0$ and $B_z$ simplifies to [13]:

$$
B_z = \frac{\mu_0 I R^2}{2 (R^2 + A^2)^{3/2}}
$$

(A.3)
Analytical description of the magnetic fields

A.1

Figure A.1: Simplified coil configuration of the Clover Leaf trap. The Gradient coils can be approximated in the calculations by straight wire segments, see Figure A.2. The direction of the currents through the coils are given. The $z$- and $r$-axes are indicated and $2A_p$, $2A_b$ and $2D$ are respectively the distances along the $z$-axis between the Pinch, Bias and Gradient coils.

A.1.1 Axial bias magnetic field

The magnetic field of the Pinch and Bias coils can be understood with a configuration of two circular loops placed at $z = \pm A$, carrying the same current $I$. Expanding the magnetic field (A.1) in a multipole polynomial expansion and comparing this expansion to the Taylor expansion of $B_z$ along the $z$-axis, we obtain to second order in dimension [34]:

$$B_r = -b_2rz + \cdots ,$$

$$B_z = b_0 + b_2(z^2 - \frac{r^2}{2})$$

$$b_0 = \frac{\mu_0 I R^2}{(R^2 + A^2)^{3/2}}$$

$$b_2 = b_0 \frac{3(4A^2 - R^2)}{2(R^2 + A^2)^2},$$

where $b_0 \equiv B_0$ and $b_2 \equiv \frac{1}{2}B'' = \frac{1}{2} \frac{\partial^2 B}{\partial r^2}$.

A.1.2 Radial quadrupole magnetic field

The radial gradient magnetic field has zero axial magnetic field both in the $z = 0$ plane and along the $z$-axis, due to the symmetry of the configuration. The approximation of the Gradient coils shown in Figure A.2b) is used to calculate the radial magnetic field generated by the Gradient coils. The magnetic field components of the eight Gradient coils are then to second order given by [34]:

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Figure A.2: Schematic diagram of the Gradient coils a), and the simplification of the Gradient coils in two steps, b) and c). Simplification b) is used to calculate the radial quadrupole magnetic field and simplification c) illustrates the essential geometry of the coils. Both simplifications a) and b) are equivalent, since the two elliptical wire segments, with radius $\rho_1$ and $\rho_2$, respectively, cancel each other. The straight wire segments thus represent the essential geometry of the Gradient coils.
A.2 Magnetic field of the MOT

The magnetic field of the MOT coils can be understood with a configuration of two circular loops placed at $z = \pm A$, carrying opposed currents $I$, analogue to the Bias and Pinch coils. For points near the origin the magnetic field is given by [1]:

$$B_z = b_1 z + b_3 \left( z^3 - \frac{3}{2} r z^2 \right) + \cdots,$$

$$B_r = -\frac{1}{2} b_1 r + b_3 \left( -\frac{3}{2} r z^2 + \frac{3}{8} r^2 z^2 \right) + \cdots,$$

where

$$b_1 = \frac{3 \mu_0 I R^2 A}{(R^2 + A^2)^{5/2}},$$

$$b_3 = \frac{5 (4 A^2 - 3 R^2)}{(R^2 + A^2)^2}. $$

The $x-$, $y-$ and $z-$component of the spherical quadrupole field of the MOT coils are now to first order equal to:

$$B_x = -\frac{1}{2} b_1 x,$$

$$B_y = -\frac{5}{8} b_1 y,$$

$$B_z = b_1 z.$$

So, contrary to the radial quadrupole field of the Gradient coils, $B_x$ is now to first order linear in $x$ and $B_y$ linear in $y$. Also $\frac{\partial B_x}{\partial x} = -2 \frac{\partial B_y}{\partial x} = -2 \frac{\partial B_y}{\partial y}.$
Appendix B

Temperature characteristic of a Gradient coil

The temperature characteristic of a Gradient coil is measured as a function of the current through the coil, in order to determine, if the watercooling is sufficient to reduce the heating of the coil to acceptable values. The surface temperature of the Gradient coil is measured with Negative Temperature Coefficient (NTC) sensors. These resistance-temperature (R-T) matched thermistors are accurate over a temperature range of −80 to +150°C. The tolerance over the temperature range of 0 to +70°C equals ±0.2°C. The temperature (T) - resistance (R) characteristic of the NTCs is depicted in Figure B.1.

The temperature is measured as a function of the current through the Gradient coil at four different positions, as shown in Figure B.2. NTC A is placed directly at the entrance of the coil. Both the current and the water stream enter the coil here. NTC B is placed at the exit of the coil. NTC C and D are, respectively, placed at an elliptic and a straight wire segment of the coil. The resistance is converted to the corresponding temperature, using the T-R characteristic of the NTC. The results are presented in Figure B.3.

The water flow through the coil equals 0.3 L/minute = 5 × 10⁻⁶ m³/s. The cross section of the coils equals $A = 1.96 \times 10^{-6}$ m². Together this yields an average flow velocity of $V = 2.55$ m/s. This means that the flow is turbulent, therefore condensation of the cooling water should be no problem. The initial temperature of the water equals 15°C.

Fitting the temperature, $T$, as a function of the current, $I$, we obtain a quadratic relation between $T$ and $I$ as expected (for the power $P = RI^2$). Also, Figure B.3 clearly shows that the temperature at the beginning of the coil (NTC A) is almost, but not quite, constant. The temperature ($T_A$) increases by $\approx 10°C$. Apparently some heat is dissipated in the cable and 'tail’ of the Gradient coil, see Figure B.2. Furthermore, the temperature at the exit of the coil (NTC B), increases very rapidly, whereas the temperature of the elliptic and linear part increases more slowly. This is also in agreement with expectations.

From Figure B.3 it is clear that, at the exit of the Gradient coil (NTC B), the temperature of the coil has increased by no less than 50°C for a current of $I = 300$ A. Such a large heating effect is unacceptable. Therefore, the flow velocity of the water through the coils in the final setup is increased with a water pump, which increases the water pressure and thus the flow velocity. The water flow

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Temperature characteristic of a Gradient coil

Figure B.1: The temperature (T) - resistance (R) characteristic of the NTCs. The x-axis has a ln-scale and the y-axis a linear scale.

Figure B.2: Schematic drawing of the Gradient coil. The positions of the four NTCs are given. NTC A is placed directly at the entrance of the coil. Both the current and the water stream enter the coil here. NTC B is placed at the exit of the coil. NTC C and D are, respectively, placed at an elliptic and a straight wire segment of the coil.
Temperature characteristic of a Gradient coil

Figure B.3: The temperature at position A, B, C and D of the Gradient coil as a function of the current through the coil.

through all the coils of the Clover Leaf trap and the MOT is now equal to 55 m/s, when we take the smallest cross section of the circuit. Due to this $\approx 20$ time larger flow, the heating in the circuit should be reduced to acceptable values.
Appendix C

Interaction of an atom with a radiation field

In a two-level atom, the ground $|g\rangle$ and excited $|e\rangle$ state can each be characterized by a stationary eigenstate of the undisturbed Hamiltonian, according to

$$|g\rangle = |a_g J_g m_g\rangle,$$

where $J_g$ is the total angular momentum quantum number, $m_g$ the quantum number which describes the projection of the total angular momentum on the quantization axis and $a_g$ a quantum number that contains all information about the eigenstate, $|g\rangle$, which is not provided by either $J_g$ or $m_g$.

Solving the time dependent Schrödinger equation, the interaction between a monochromatic radiation field and a two-level atom can be found. The matrix element which describes this interaction is:

$$\langle e| - \vec{E}(t) \cdot \vec{d}|g\rangle,$$

where $\vec{d}$ is the dipole operator of the atom and $\vec{E}(t)$ the radiation field. When choosing a suitable basis ($\vec{z}, \frac{1}{\sqrt{2}}(\vec{x} + i\vec{y}), \frac{1}{\sqrt{2}}(\vec{x} - i\vec{y})$), the dipole operators will behave in a similar manner as the spherical wave functions, $Y_{L,M}(\theta, \phi)$ under rotations. The transition matrix elements of the dipole operator (C.2) are now equal to:

$$\langle a_e J_e m_e | d_{LM} | a_g J_g m_g \rangle.$$

Here $L$ and $M$ are the quantum numbers of the spherical wave function $Y_{L,M}$. For linearly polarized ($\pi$) light ($\vec{d} = -e \cdot \vec{z}$), $L = 1$, $M = 0$. For right hand circularly polarized ($\sigma^+$) and left hand circularly polarized ($\sigma^-$) light, $L = 1$, $M = 1$ and $L = 1$, $M = -1$, respectively.

According to the Wigner Eckart theorem, these transition matrix elements (C.3) can be written as the product of a geometrical factor and a reduced matrix element, the latter being independent of the magnetic quantum numbers $m_e$ and $m_g$ [15]:

$$\langle a_e J_e m_e | d_{LM} | a_g J_g m_g \rangle = \frac{(J_g m_g LM | J_e m_e)}{(2 J_e + 1)^{1/2}} \langle a_e J_e | d_L | a_g J_g \rangle.$$

The term $(J_g m_g LM | J_e m_e)$ is the Clebsch-Gordon coefficient, which is always real. The Clebsch-Gordon coefficient represents the probability amplitude that $J_g$ and $L$ are coupled into a resultant
Interaction of an atom with a radiation field

Figure C.1: The relative transition probability for $J_g = 2 \leftrightarrow J_e = 3$ transition. Dividing the coefficients by 105, yields the correct absolute value of the transition probability (C.5). According to this scheme the transition probability for the Ne$^*$ $|^3P_2, m_J = 2 \leftrightarrow Ne^{**} |^3D_3, m_J = 3)$ transition is equal to $\frac{15}{105} = 0.1429$.

Angular momentum $J_e$ with projection $m_e$. The transition matrix elements (C.3) are directly proportional to these Clebsch-Gordon coefficients and the relative transition probability is directly proportional to their square [15]:

$$
\frac{(J_g m_g L M |J_e m_e|^2}{(2J_e + 1)} = \frac{(J_g m_g L - M |J_e m_e|^2}{(2J_e + 1)}.
$$

(C.5)

These transition probabilities are given in Figure C.1 for the Ne$^*$ $|^3P_2 \leftrightarrow Ne^{**} |^3D_3$) transition.

The second term in equation (C.4) is the so-called reduced matrix element which contains the physical information about the radial part of the wave function. For the Ne$^*$ $|^3P_2, m_J = 2 \leftrightarrow Ne^{**} |^3D_3, m_J = 3)$ transition it is equal to $3.617 \times 10^{-10}$ m.
Appendix D

Sub-Doppler cooling

D.1 Polarization gradients

Figure D.1 shows schematically the polarization gradients and the corresponding light shifted ground state sublevels for a $J_g = 1/2 \leftrightarrow J_e = 3/2$ atomic transition in the $\sigma^+ - \sigma^-$ configuration in a one-dimensional molasses. In the $\sigma^+ - \sigma^-$ configuration, the polarization vector rotates when one moves along the standing wave, but it keeps the same ellipticity (Figure D.1a). In $z = 0$, the total electric field is linearly polarized along $\epsilon_y$. Moving along the $z-$axis the polarization of the electric field rotates and forms a helix with pitch $\lambda$. The laser polarization is always linear and the laser intensity is the same for all $z$ (Figure D.1a). As a result the light shifted energies, which are proportional to the light intensity, do not vary as a function of $z$ (Figure D.1c).

D.2 Induced Orientation effect

The induced orientation effect is based on motion induced population differences between the Zeeman sublevels $|J, m_J\rangle$, and occurs in the $\sigma^+ - \sigma^-$ configuration. Looking at Figure C.1, it is clear that the transition probability between sublevels differs. Since the light shift is directly proportional to the intensity of the transition, the Zeeman sublevels will have different light shifts. Although the laser intensity and thus the light shift does not vary as a function of $z$, the wave functions do. As a result nonadiabatic couplings could occur among the various Zeeman sublevels undergoing different light shifts.

Imagine an atom at rest at $z = 0$ in the $\sigma^+ - \sigma^-$ configuration. Figure D.1 shows that the total electric field is polarized along $\vec{f}$. Optical pumping with $\pi$ polarized light will concentrate atoms in $|^3P_2, m_J = 0\rangle_y$, because the transition probabilities for the transitions $|2, -2\rangle_y \rightarrow |2, -1\rangle_y, |2, -1\rangle_y \rightarrow |2, 0\rangle_y, |2, 1\rangle_y \rightarrow |2, 0\rangle_y$ and $|2, 2\rangle_y \rightarrow |2, 1\rangle_y$, are greater than the transition probabilities of the opposite processes (Figure C.1). Figure C.1 also clearly shows that the optical pumping rate is equal for transitions starting from the $|2, -2\rangle_y$ and $|2, 2\rangle_y$ states. The same holds for the transitions starting from $|2, -1\rangle_y$ and $|2, 1\rangle_y$. Therefore these pairs of atomic levels will undergo the same light shift $\Delta'_{m_J}$. Moreover, the $\pi$ transition starting from $|2, 0\rangle$ is $9/8$ times more intense than the transitions starting from $|2, \pm 1\rangle_y$ and $9/5$ times more intense than the transitions starting from $|2, \pm 2\rangle_y$. Since the light shift is directly proportional to the intensity of the transition, we obtain $\Delta'_0 = 9/8\Delta'_{\pm 1} = 9/5\Delta'_{\pm 2}$. 
Figure D.1: Schematic view of the polarization gradients and the corresponding light shifted ground state sublevels for a \( J_g = 1/2 \leftrightarrow J_e = 3/2 \) atomic transition in the \( \sigma^+ - \sigma^- \) in a one-dimensional molasses. (a) Polarization gradients in the \( \sigma^+ - \sigma^- \) configuration: Two counter propagating \( \sigma^+ \) and \( \sigma^- \) waves, result in a linear polarization that rotates in space along the propagation axis. (b) Light shifted ground state Zeeman sublevels for the \( \sigma^+ - \sigma^- \) configuration: The light shifted energies do not vary with \( z \).

Although the laser intensity and thus the light shifts do not vary as a function of \( z \), the wavefunctions do. For the light shifted Zeeman sublevels \( |J, m_J\rangle \) are the eigenstates of the component of \( \mathbf{J} \) along the rotating laser polarization \( \mathbf{e}_Y \). Now we consider an atom moving along the \( z \)-axis with velocity \( v \). From the atoms point of view the laser polarization \( \mathbf{e}_Y \) rotates around \( z \), making an angle \( \phi = -kz = -kv t \) with the \( y \)-axis. In a rotating frame in the atoms rest frame in which the laser polarization has a fixed direction, an extra inertial field will appear as a result of the rotation. This inertial term is a fictitious magnetic field parallel to the rotation axis \( z \) with an energy given by [7]:

\[
V_{\text{rot}} = kv J_z. \tag{D.1}
\]

Assuming that \( |\Delta'| \gg \Gamma' \), so that the energy splitting between the \( |^3P_2\rangle \) levels is much larger than their widths, and \( |\Delta'| \gg kv \), so that the Doppler shift is much smaller than the light shifts of the \( |^3P_2\rangle \) levels, the effect of \( V_{\text{rot}} \) can be treated with perturbation theory. Due to the couplings between the \( |^3P_2\rangle \) states, induced by the perturbation \( V_{\text{rot}} \), the levels are shifted to second order in \( kv/\Delta' \), and more important, the wavefunctions of the Zeeman sublevels mix to first order in \( kv/\Delta' \) [7]. Or in other words, the perturbed eigenstates of \( V_{\text{rot}} \) are linear combinations of all sublevels which are coupled by \( V_{\text{rot}} \) to these sublevels. As a result the populations of the eigenstates of \( J_z, |J, m_J\rangle_z \), are no longer equal as they were in the unperturbed \( |J, m_J\rangle_y \) states [7].

This motion induced population difference between the sublevels causes an unbalance in the radiation pressure. Imagine an atom moving from the left to the right (\( v > 0 \)), in a red detuned optical molasses. A cumbersome analysis shows that the \( |J, -m_J\rangle_z \) state is then more populated than the \( |J, m_J\rangle_z \) state [7]. Looking at Figure C.1 it is clear that there is a much greater probability that
an atom in \(|J,-m_J\rangle_z\) will absorb a \(\sigma^-\) photon propagating towards \(z < 0\) than it will absorb a \(\sigma^+\) photon propagating towards \(z > 0\). As a consequence the atom will scatter more counterpropagating \(\sigma^-\) photons than copropagating \(\sigma^+\) photons, and the velocity of the atom will be damped. The reverse conclusions can be drawn for \(|J,m_J\rangle_z\) states.

The mean force acting on an atom is now equal to the difference in the number of \(\sigma^+\) and \(\sigma^-\) photons scattered per unit time, times the photon momentum \(\hbar k\), and can be shown to be given by [7]:

\[
\vec{F} = -\beta \vec{v} \sim -\hbar k^2 \frac{\Gamma'}{\Delta'} \vec{v}.
\]  

\[\text{(D.2)}\]

For \(\delta = -5\Gamma\) and \(s_0 = 0.5\) (\(\Omega = 5\Gamma\)), the transition rate (3.11) is equal to: \(\Gamma' = -2.05\ (2\pi)\ 10^4\ \text{Hz}\). Using equation (3.10), we obtain for the light shift \(\Delta' = -10.1\ (2\pi)\ 10^4\ \text{Hz}\). The friction constant \(\beta\) can then be estimated at: \(\beta \sim -2.06 \times 10^{-21}\ \text{kg/s}\).

The spring constant in the low field region around the center of the trap is due to the induced orientation effect. As a result of the presence of a small magnetic field, the velocity to which the atoms are cooled is shifted to a velocity \(v_B\), determined by [1]:

\[
\vec{v}_B = -\frac{gJ_\delta \mu_B B}{\hbar k},
\]

\[\text{(D.3)}\]

where \(B = \frac{\partial B}{\partial z} x\). The damping of the atom velocity towards \(\vec{v}_B\) can be expressed as follows:

\[
\vec{F} = -\beta (\vec{v} - \vec{v}_B) = -\beta \vec{v} - \kappa \vec{z},
\]

\[\text{(D.4)}\]

where \(\beta\) is defined by equation (D.2). From equation (D.4), we obtain the spring constant \(\kappa_{ind}\) [7]:

\[
\kappa_{ind} = \frac{gJ_\delta \mu_B \partial B}{\hbar k} \beta.
\]

\[\text{(D.5)}\]

For the \(\text{Ne}^* \left| ^3P_2, m_J = 2 \right\rangle \leftrightarrow \text{Ne}^{**} \left| ^3D_3, m_J = 3 \right\rangle\) transition with a detuning of \(\delta = -5\Gamma\), a saturation parameter of \(s = 0.5\) and a axial magnetic field gradient of \(1\ \text{G/mm}\), the spring constant is equal to \(\kappa_{ind} = 2.8 \times 10^{-18}\ \text{N/m}\).

The time necessary to cool the atoms to the origin is given by [15]:

\[
\tau = \frac{2\gamma}{\omega_{osc}^2},
\]

\[\text{(D.6)}\]

where \(\gamma = \beta/m\) and \(\omega_{osc} = \sqrt{k/m}\). For the above described situation this yields: \(\tau_{ind} = 1.5\ \text{ms}\).

As an estimate for the diffusion coefficient \(D\), we use the exact solution of the diffusion coefficient for the \(J_g = 1 \leftrightarrow J_e = 2\) transition in the low power limit [7]:

\[
D_{ind} = \left[ \frac{36}{171} + \frac{1}{(4\delta^2/5\Gamma^2)} \right] \frac{58}{170} \hbar^2 k^2 \Gamma s.
\]

\[\text{(D.7)}\]

For the \(\text{Ne}^* \left| ^3P_2, m_J = 2 \right\rangle \leftrightarrow \text{Ne}^{**} \left| ^3D_3, m_J = 3 \right\rangle\) transition with a detuning of \(\delta = -5\Gamma\) and a saturation parameter of \(s_0 = 0.5\), the diffusion constant is now equal to: \(D_{ind} = 1.22 \times 10^{-40}\ \text{kg s}^{-2}\). Substituting \(D_{ind}\) and \(\beta_{ind}\) into equation (3.8) yields: \(T_{sub} = 4.3\ \mu\text{K}\).
Appendix E

MOT measurements

Table E.1 gives an overview of the measured number of particles $N$ in the MOT, the volume $V$ of the confined atom cloud, the particle density $n$ in the MOT, the time constant $\tau_{\text{ion}}$ for loss due to ionization and the ionization rate constant $\beta_{\text{ion}}$ as a function of the detuning of the MOT laser beams, for different MOT magnetic field gradients.
### MOT measurements

Table E.1: The number of particles $N$ in the MOT, the volume $V$ of the confined atom cloud, the particle density $n$ in the MOT, the time constant $\tau_{\text{ion}}$ for loss due to ionization and the ionization rate constant $\beta_{\text{ion}}$ are determined from the fluorescence intensity as a function of the detuning of the MOT laser beams, for different MOT magnetic field gradients.

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<th>$B^a$ (G/mm)</th>
<th>$\delta_{\text{laser}}^b$ (G)</th>
<th>$N$ $(10^6)$</th>
<th>$V$ $(10^9$ cm$^3$)</th>
<th>$n_0$ $(10^{10}$ cm$^{-3}$)</th>
<th>$\tau_{\text{ion}}$ (s)</th>
<th>$\beta_{\text{ion}}$ $(10^{-10}$ cm$^3$ s$^{-1}$)</th>
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<td>3.34 ± 0.02</td>
<td>0.038 ± 0.006</td>
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<td>0.090 ± 0.002</td>
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<td>0.093 ± 0.007</td>
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<td>11 ± 2</td>
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<td>1.3 ± 0.3</td>
<td>0.036 ± 0.005</td>
<td>21 ± 7</td>
</tr>
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</table>

$^a\Delta B' = 0.0033$ G/mm

$^b\Delta \delta = 2$ MHz $= 0.24\Gamma$
Appendix F

Molecule-fixed frame

There are two coordinate systems that are useful in the description of atomic collisions: the lab-fixed frame \((x, y, z)\) and the molecule-fixed frame \((x', y', z')\). The lab-fixed frame does not change its orientation in time, the molecule-fixed frame is locked to the molecule.

In collision calculations, molecular states are usually defined with respect to the molecule-fixed frame because the symmetry labels identifying these states are related to symmetry operations in the molecule-fixed frame. In the experiment, however, when the distribution of the atoms over the different states is important, the atomic states are usually defined with respect to the lab-fixed frame [38].

Figure F.1 shows the orientation of the molecule-fixed frame relative to the lab-fixed frame. The origin of both frames is chosen to coincide with the center of mass of the molecule. The orientation of the molecule-fixed frame with respect to the lab-fixed frame can be given in terms of three Eulerian angles \(\alpha, \beta, \gamma\) [38]. Assuming that the two frames initially coincide (internuclear axis \(z'\) aligned along the lab-fixed \(z\) axis), the three following rotations are performed to obtain the orientation of the internuclear axis. First, the molecule-fixed frame is rotated over an angle \(\gamma\) around the lab-fixed \(y\)-axis. Then the molecule-fixed frame is rotated over \(\beta\) around the lab-fixed \(y\)-axis. To conclude, the molecule-fixed frame is rotated over an angle \(\alpha\) around the lab-fixed \(z\)-axis.

Figure F.1 also shows the vector diagram of Hund's case (c) coupling. For heavy nuclei the spin-orbit interaction is often stronger than the coupling of either the electronic orbital angular momentum \(L\) or the electronic spin angular momentum \(S\) to the internuclear axis. Therefore, \(L\) and \(S\) first add vectorially to form the electronic total angular momentum \(j\), which then couples to the internuclear axis to make the projection \(\Omega\). The rotational angular momentum \(I\) then forms together with \(\Omega\) the total angular momentum \(J\) [41].
Figure F.1: Orientation of the molecule-fixed frame \((x', y', z')\) with respect to the lab-fixed frame \((x, y, z)\). Also the vector diagram of Hund's case (c) coupling is given.
Appendix G

Technology assessment

The main interest of Bose-Einstein condensates, laser cooling and trapping of atoms lies in fundamental research. However, an increasing number of applications of laser cooling, trapping of atoms and Bose-Einstein condensates is arising. Atomic clocks have already been in use for quite some time. Atomic clocks are much more accurate than any other known timekeeping devices. In atomic clocks, time is related to an atomic transition observed in a laser cooled atomic beam. The accuracy of the atomic clock can be increased by a factor $100 - 1000$ when cold atoms are used. The accuracies of atomic clocks led to a redefinition of the SI second as the duration of $9192631770$ periods of the hyperfine transition of the ground state $^{133}\text{Cs}$ atom [18].

Another emerging application of Bose-Einstein condensates, is the atom laser. Stimulated Raman transitions between magnetic sublevels can be used to transfer atoms from a magnetically trapped to an untrapped state and to impart a well-defined momentum to the output coupled condensate. By using higher order Raman transitions, it is possible to impart any momentum $2\pi n h \vec{k}$, where $n$ is an integer, to the atoms. In this way it is possible to choose the energy of the extracted De Broglie wave, producing a highly tunable and highly collimated quasi-continuous laser [12].

Another application being intensively studied is atom interferometry. An atom interferometer splits an atom into two waves separated in space. The two parts of the atom are then recombined and interfere with each other. The resulting interference effects can be used to measure physical phenomena, like gravity, with high sensitivity [5].

The basic principles of atom trapping can also be applied to micron sized particles, such as live bacteria. An intense focused laser beam can be used to manipulate live cells without afflicting any damage. The intense electric field at the center of the focused laser beam polarizes the particle and will draw it into the region of the highest laser intensity. Using this 'optical tweezer', chromosomes have been manipulated inside a cell nucleus. Even manipulation of a single DNA molecule has been demonstrated [5]. The use of these optical tweezers will have a large impact on biology, chemistry and medicine in the near future.

This list is not exhaustive and new applications are still arising. Summarizing, the field of laser cooling, trapping of atoms and Bose-Einstein condensates is a very promising field, not only in fundamental physics but also in technological applications.